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VERIFICATION OF A TOXIC ORGANIC SUBSTANCE TRANSPORT AND BIOACCUMULATION MODEL

by

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16. ABSTRACT

A field verification of the Toxic Organic Substance Transport and Bioaccumulation Model (TOXIC) was conducted using the insecticide dieldrin and the herbicides alachlor and atrazine as the test compounds. The test sites were two Iowa reservoirs. The verification procedure included both steady-state analyses and quasi-dynamic simulations using time-variable flows and pollutant loadings along with model coefficients derived from laboratory and literature data. Laboratory measurements were used in simulations of alachlor, atrazine and dieldrin, and model predictions were well within an order of magnitude of field observations. For the herbicide alachlor, for example, laboratory protocol measurements were used directly in model simulations with excellent agreement between model predictions and measured concentrations

The TOXIC model, therefore, was considered to be field verified. Moreover, the successful field verification supports the validity of EPA's Exposure Analysis Modeling System (EXAMS), which handles pollutant transport and transformation kinetics in an almost identical manner.

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FOREWORD

As environmental controls become more costly to implement and the penalties of judgment errors become more severe, environmental quality management requires more efficient analytical tools based on greater knowledge of the environmental phenomena to be managed. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Technology Development and Applications Branch develops and tests management and engineering tools to help pollution control officials achieve water quality goals.

Concern about environmental exposure to synthetic organic compounds has increased the need for reliable techniques to predict the behavior of chemicals entering natural waters as a result of the manufacture, use, and disposal of commercial products. In response, mathematical models have been developed to aid in evaluating the environmental consequences of pollutant exposure. An essential step in the development and use of these models is field verification. This report describes a recent study in which the Toxic and Organic Substance Transport and Bioaccumulation Model (TOXIC) predicted pesticide concentrations that were well within an order of magnitude of levels actually measured in two Iowa reservoirs. This successful field verification of TOXIC also supports the use of EPA's Exposure Analysis Modeling System, which incorporates similar modeling procedures.

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ABSTRACT

The model TOXIC (and versions thereof) was calibrated for the insecticide dieldrin and the herbicides alachlor and atrazine using data from Iowa reservoirs. Steady state analyses and quasi-dynamic simulations with time-variable flows and loadings were accomplished. Model coefficients were derived from laboratory data and in some cases literature data.

For the herbicide alachlor, laboratory protocol measurements were used directly in model simulations with excellent agreement between model predictions and measured concentrations. Thus the model may be considered field-validated. Laboratory measurements were used in simulations of alachlor, atrazine and dieldrin, and results were well within an order-of-magnitude of field data.

One of the most important aspects of the dieldrin simulations was the choice of time and space scales. Especially in quasi-dynamic applications, where one variable varies in time and space while another is held constant, averaging problems arise. To simulate both the exposure concentration and mass fluxes accurately, one must use a fully dynamic, spatially variable model in which flow, suspended solids, toxicant concentration, pH, and other state variables are functions of time and space. Fortunately most applications do not require such accuracy, and we may settle for steady state or quasi-dynamic models such as TOXIC. TOXIC was utilized in a management decision by the Iowa Conservation Commission to lift the ban on commercial fishing in Coralville Reservoir in 1979.

Sediment has been a small net source of dieldrin to the water column of Coralville Reservoir, especially important under low flow conditions. Coralville Reservoir contains approximately 50 kg of dieldrin in the sediment. It will take 6-10 more years to achieve less than detectable (<0.002 μg/ℓ) dieldrin in the water column, primarily due to continued inflow as well as sediment desorption.

Lastly, field bioconcentration factors when normalized on a lipid basis were approximately equal to laboratory-derived bioconcentration factors similarly weighted. The bioconcentration factors were also proportional to the octanol water partition coefficient. Bioconcentration is the primary mode of pesticide uptake in Coralville Reservoir and food items are generally of less importance.

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CHAPTER I

DIELDRIN IN CORALVILLE RESERVOIR: MODEL DEVELOPMENT AND CALIBRATION

INTRODUCTION

Agricultural usage of pesticides in Iowa is widespread, particularly grass and broadleaf herbicides and row crop soil insecticides. One of the insecticides widely used for control of the corn rootworm and cutworm from 1960 to 1975 was the chlorinated hydrocarbon, aldrin. Aldrin is microbially metabolized to its very persistent epoxide, dieldrin. Dieldrin is itself an insecticide of certain toxicity and is also a very hydrophobic substance of limited solubility in water (0.25 ppm) and low vapor pressure (2.7×10^{-6} mm Hg @ 25°C). It is known to bioaccumulate to levels as high as 1.6 mg/kg wet weight in edible tissue of Iowa catfish [1], Table I-1.

Aldrin application in Iowa during the mid-1960's amounted to some 2.94×10^{6} kg/yr on 5.0 million acres (2×10^{10} m^2). However, the corn rootworm grew increasingly resistant to aldrin and, after 1967, usage decreased across the state by approximately one-half. Finally, the pesticide was banned in 1975 and very little was applied after 1976. Although aldrin was no longer labeled, dieldrin residues in excess of the Food and Drug Administration "action" level (0.3 mg/kg wet edible tissue) were recorded for Coralville Reservoir fishes, and commercial fishing was banned in 1975. The problem was to determine the fate and transport of the pesticide dieldrin and to assess when the residual concentrations would be acceptable for commerical fishing.

Coralville Reservoir is a mainstream impoundment of the Iowa River in Eastern Iowa. It drains approximately 7978 km^2 of prime Iowa farmland and receives extensive agricultural runoff with 90% of its drainage basin in intensive agriculture. It is a variable-level, flood control and recreational reservoir which has undergone considerable sedimentation since it was created in 1958. At conservation pool (680 ft. above msl), the Reservoir has a capacity of 4.69×10^{7} m^3, a surface area of 1.98×10^{7} m^2, a mean depth of approximately 2.44 m, and a mean detention time of 14 days. In 1958, the capacity at conservation pool was 6.63×10^{7} m^3.

Several models have been developed to assess the fate and transport of agricultural chemicals including the Agricultural Runoff Model (ARM) [2], the Nonpoint Source Pollution Model (NPS) [3], the Stanford Research Institude Kinetic Model (SRI) [4], and the Exposure Analysis Modeling System (EXAMS) [5]. The first two models are primarily designed to simulate the delivery of soil particles and agricultural chemicals to the edge of the stream bank. They make extensive use of the modified Universal Soil Loss Equation and knowledge of the chemical partitioning between soil and water, together with a given flood hydrograph. The SRI and EXAMS models are

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kinetic formulations which describe the chemical, physical and biological reactions which a pesticide can undergo once it reaches the water body. Chemical hydrolysis, volatilization, photolysis, and biological degradation comprise the reactions considered in these models. Instantaneous adsorption and desorption equilibrium is also assumed. Relative importance of the pathways of pesticide fate (hydrolysis, volatilization, photolysis, biological degradation, oxidation, and sorption) may be assessed in the laboratory [4].

Previous models have not been extensively verified with field data, and they have not combined fate and transport modeling with the biological effects (bioconcentration). In this research, a pesticide transport and bioconcentration model is developed and applied to Coralville Reservoir to assess the fate and effects of dieldrin in the ecosystem. Results have aided the Iowa Conservation Commission in their decision to lift the commercial fishing ban on November 7, 1979.

MODEL DEVELOPMENT

A schematic of pesticide fate and transport within a reservoir is presented in Fig. I-1. The solid lines are in accordance with the SRI model formulation [4]. Modifications in both the kinetics and transport (which might add increased realism to the model) are represented by dashed lines. A two-compartment or "pond" representation of the reservoir was assumed since there exist few in-reservoir data with which to calibrate a multi-compartment model. Fig. I-2 gives the physical configurations of the completely mixed compartments utilized in the model. Coralville Reservoir dimensions were used in the pond configuration for model calibration, and simulations were later performed using the lake configuration as well.

Although the field data reflect individual storm events, the goal here was to represent annual average concentrations and mass flows. Therefore, constant annual average inflow and outflow rates were assumed, together with an average annual volume for the reservoir. Coralville Reservoir does not thermally stratify to any great extent, so the failure to include a hypolimnion compartment in the pond configuration is not viewed as a serious problem.

In addition to chemical reaction pathways, fish uptake and depuration (excretion and metabolism) was included in the model. The bioconcentration part of the model formulation is depicted separately in Fig. I-3. Biouptake is proportional to the product of the fish biomass and the dissolved pesticide concentration. Pesticide is removed by the fish as water passes the gill membrane. Biouptake from sediment and/or food (prey) items could also be included in this portion of the model. Here it is assumed that the pesticide residue is metabolized within the fish, but in some cases it may be necessary to recycle the depurated pesticide as a dissolved input.

Mass Balance for Pesticides in Reservoirs

The distribution of pesticides in reservoirs is established by application of the principle of continuity or mass balance. Each phase, the dissolved and particulate, is analyzed separately, taking into account the interaction with the other. Thus for the dissolved component, the mass balance includes various reaction pathways [4] in addition to the inflow and outflow. The basic differential equation can be written to include the sum of the first order or pseudo-first order reactions (hydrolysis, biological degradation, biological uptake, photolysis, and volatilization) as well as adsorption and desorption kinetics as a function of particle size distribution:

$$\frac{dC}{dt} = \frac{W_c}{V} - \frac{C}{t_o} - \sum_{i=1}^{4} k_i C - \sum_{j=1}^{n} k_{f_j} M_j C + \sum_{j=1}^{n} k_{r_j} C_{p_j} \qquad (1)$$

in which

V = reservoir volume, L^3

W_c = rate of mass input of the dissolved component, M/T

t_o = mean hydraulic detention time, T

C = dissolved chemical concentration, M/L^3

$\sum_{i=1}^{4} k_i$ = sum of the first order decay rate constants including the following:

$k_1 = k_1'$ [Bacteria] = pseudo-first order biological degradation rate constant, T^{-1}

$k_2 = k_2'\,[OH^-]$ = base catalyzed, pseudo-first order hydrolysis rate constant, T^{-1}

$k_3 = k_3'$ (quantum yield) = first order direct photolysis rate constant, T^{-1}

k_4 = first order volatilization rate constant, T^{-1}

$\sum_{j=1}^{n} k_{f_j}$ = sum of the adsorption rate constants for the j^{th} size fraction, n total fractions, $L^3/M\text{-}T$

M_j = suspended solids concentration in the j^{th} size fraction, M/L^3

$\sum_{j=1}^{n} k_{r_j}$ = sum of the desorption rate constants for the j^{th} size fraction, n total fraction, T^{-1}

C_{p_j} = particulate chemical concentration due to the j^{th} size fraction, M/L^3.

If we do not partition the suspended solids concentration into various size fractions or if only one size fraction is active in sorbing the chemical of interest, then Equation 1 reduces to:

$$\frac{dC}{dt} = \frac{W_c}{V} - \frac{C}{t_o} - \Sigma kC - k_f\,MC + k_r\,C_p \qquad (2)$$

in which

Σk = overall decay coefficient of the dissolved chemical, T^{-1}

For the particulate chemical concentration in the j^{th} size fraction:

$$\frac{dC_{p_j}}{dt} = \frac{W_{p_j}}{V} - \frac{C_{p_j}}{t_o} - k_{s_j}\,C_{p_j} - k_{r_j}\,C_{p_j} + k_{f_j}\,M_j\,C \qquad (3)$$

in which

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W_{p_j} = rate of mass input of the particulate adsorbed chemical of size fraction j, M/T

k_{s_j} = sedimentation coefficient of the j^{th} size fraction, T^{-1}

Summing the total over j size fractions or if only one size fraction is considered, equation (1) reduces to:

$$\frac{dC_p}{dt} = \frac{W_p}{V} - \frac{C_p}{t_o} - k_s\,C_p - k_r\,C_p + k_f\,MC \qquad (4)$$

in which

k_s = overall sedimentation coefficient, T^{-1}

k_r = overall desorption rate constant, T^{-1}

k_f = overall adsorption rate constant, $L^3/M\text{-}T$

Adding Equations 2 and 4 cancels the adsorption and desorption terms and yields the rate of change of the total concentration C_T in terms of the dissolved and particulate:

$$\frac{dC_T}{dt} = \frac{W(t)}{V} - \frac{C_T}{t_o} - \sum kC - k_s\,C_p \qquad (5)$$

in which

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C_T = total concentration = $C + C_p$

W = total mass input

The sorption coefficients k_f and k_r are usually orders of magnitude greater than the decay and transfer coefficients of the dissolved and particulate phases. Thus instantaneous local equilibrium is achieved between the two phases - i.e. the rates of transfer and decay are so low that, comparatively, liquid-solid phase equilibrium is achieved very rapidly. The concentrations C and C_p may be replaced by their equivalents in terms of C_T providing that the adsorption isotherm is known and that equilibrium is achieved. Linear adsorption isotherms have been reported elsewhere [6].

$$r = K_p\, C \qquad (6)$$

in which

K_p = linear adsorption partition coefficient, $(M/M)/(M/L^3)$

r = amount of pesticide adsorbed per unit mass of dry sediment, M/M

It follows that C and C_p may be expressed in terms of C_T under conditions of local equilibrium:

$$C = \frac{C_T}{(1 + K_p\, M)} \qquad (7)$$

$$C_p = \frac{C_T\, K_p\, M}{(1 + K_p\, M)} \qquad (8)$$

Substituting for C_p and C from the above relationships into Equation 5 the mass balance differential equation is:

$$\frac{dC_T}{dt} = \frac{W(t)}{V} - \frac{C_T}{t_o} - \frac{\Sigma k}{1 + K_p\, M}\, C_T - \frac{k_s\, K_p\, M}{1 + K_p\, M}\, C_T \qquad (9)$$

which, under steady-state conditions may be expressed as:

$$C_T = \frac{W/V}{\dfrac{1}{t_o} + \dfrac{1}{1 + K_p M}\left[\Sigma k + K_p M k_s\right]} \qquad (10)$$

Equation 9 is written for only one water compartment with sedimentation of suspended solids into the sediment compartment. It is straightforward to

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extend the analysis to a number of compartments (such as the lake configuration of Fig. I-2) with interflow and bulk dispersive transport between compartments. The equations are linear and may be solved analytically or numerically.

Bioaccumulation Model

The bioconcentration model follows the simple kinetics of Fig. I-3. The total pesticide concentration is the sum of the particulate plus the dissolved concentrations, with instantaneous sorptive equilibrium assumed. The total pesticide mass balance equation is identical to Equation 9 except it is written more concisely with fractions:

$$\frac{dC_T}{dt} = \frac{W(t)}{V} - \frac{C_T}{t_o} - (\Sigma k)f_1\, C_T - k_s\, f_2\, C_T \qquad (11)$$

in which

$$f_1 = \frac{C}{C_T} = \frac{1}{(1 + K_p\, M)} = \text{fraction of dissolved pesticide}$$

$$f_2 = \frac{C_p}{C_T} = \frac{K_p M}{(1 + K_p\, M)} = \text{fraction of particulate pesticide}$$

The mass balance for the concentration of pesticides tied up in fish biomass per unit volume of water, C_F, is:

$$\frac{dC_F}{dt} = k_1\, f_1\, C_T - k_d\, C_F \qquad (12)$$

in which

k_1 = biouptake rate constant, $\frac{\text{liters filtered}}{\text{kg fish-day}}\ \frac{\text{kg fish}}{\text{liter}}$, T^{-1}

k_d = depuration rate constant, T^{-1}

$$k_d = \frac{k_1(\text{dissolved fraction})}{(\text{Biomass})\ (\text{Fish Partition})} = \frac{(k_1/\text{day})\ (f_1)}{\frac{(\text{kg fish})}{\ell}\ \frac{(\mu g/kg)}{\mu g/\ell}}$$

If one divides Equation 12 by the fish biomass, a final bioaccumulation or fish residue equation results:

defining: $\frac{dF}{dt} = (k_1 f_1 C_T/B) - k_d F$ (13)

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F = whole body fish residue level, M/M wet weight

B = fish biomass concentration, M/L^3 wet weight

The bioconcentration factor (BCF) between pesticide residue in whole fish and the dissolved concentration is the ratio of the biouptake rate constant to the depuration rate constant divided by the fish biomass, k_1/k_dB. If pesticide is not metabolized in the fish, Fig. I-3 and Equation 13 are modified to reflect excretion of pesticide back into the dissolved phase.

Equations 11 and 13 may be solved analytically for constant coefficients and simple pesticide loading functions, W(t), or they may be integrated numerically. In the case of a pesticide ban, the W(t) might typically decline in an exponential manner due to degradation by soil organisms. For an exponentially declining loading function at rate ω, the analytical solutions to Equations 11 and 13 are:

$$C_T = C_{T_o} e^{-\delta t} + \frac{C_{Tin_o}}{\varepsilon} (e^{-\omega t} - e^{-\delta t}) \qquad (14)$$

$$F = F_o e^{-k_d t} + \frac{k_1 f_1}{B} \left\{ \frac{C_{T_o}}{\gamma} e^{-\delta t} + \frac{C_{Tin_o}}{\varepsilon\theta} e^{-\omega t} - \frac{C_{Tin_o}}{\varepsilon\gamma} e^{-\delta t} \right\}$$

$$- \frac{k_1 f_1}{B} e^{-k_d t} \left\{ \frac{C_{T_o}}{\gamma} + \frac{C_{Tin_o}}{\varepsilon\theta} - \frac{C_{Tin_o}}{\varepsilon\gamma} \right\} \qquad (15)$$

in which

C_{T_o} = initial total pesticide concentration in lake, ML^{-3}

C_{Tin_o} = initial total pesticide inflow concentration, ML^{-3}

ω = rate of exponentially declining inflow concentration, T^{-1}

$\alpha = (\Sigma k)f_1 + k_1 f_1 + k_s f_2$, T^{-1}

$\gamma = k_d - \alpha - (1/t_o)$, T^{-1}

$\delta = \alpha + (1/t_o)$, T^{-1}

$\varepsilon = \alpha t_o + 1 - \omega t_o$, dimensionless

$\theta = k_d - \omega$, T^{-1}

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The steady state solution to Equations 11 and 13 reduces to Equation 10 for the total pesticide concentration. For the fish residue level at steady state, the solution to Equation 13 simply yields the fish partition coefficient times the equilibrium dissolved pesticide concentration.

Multicompartment Solutions

Multicompartment solutions of Equations 11 and 13 must include interflows and bulk dispersion as well as an assumption regarding suspended solids and fish biomass distribution. For each constant volume compartment:

$$V \frac{dC_T}{dt} = \sum Q_a C_a - \sum Q_b C_T - K_{da} f_1 C_T V - (k_s + k_{pa}) f_2 C_T V + K_{sa} f_2 C_a V_a + \frac{EA}{\ell}(C_a - C) \qquad (16)$$

where

V = compartment volume (m^3)

C_T = total pesticide concentration of the compartment ($\mu g/\ell$)

t = time (d)

Q_a = inflow of water from adjacent compartment (m^3/d)

Q_b = outflow of water to adjacent compartments (m^3/d)

C_a = total pesticide concentration in the adjacent compartment ($\mu g/\ell$)

f_1 = fraction of the total pesticide in the dissolved phase

f_2 = fraction of the total pesticide in the particulate phase

K_{da} = reaction rate constant for the dissolved phase (d^{-1})

K_{pa} = reaction rate constant for the particulate phase (d^{-1})

k_s = settling rate constant of the compartment (d^{-1})

k_{sa} = settling rate constant from the above compartment (d^{-1})

E = bulk dispersion coefficient for adjacent compartments (m^2/d)

A = surface area between two adjacent compartments (m^2)

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ℓ = mixing length between midpoints of adjacent compartments (m)

V_a = volume of above compartment (m^3)

The general mass balance equation for the compartments can be reduced to a general matrix equation, Equation 17.

$$\frac{d\{Cj\}}{dt} = \left[\frac{Q_{i,j}}{V_j}\right]\{C_i\} - \left[\frac{Q_{i,j}}{V_j}\right]\{C_j\} - \left[f_{1,j}\,K_{da} + f_{2,j}\,k_{s,j} + f_{2,j}\,K_{pa}\right]$$

$$\{C_j\} + \left[f_{2,i}k_{s,i}\,\frac{V_i}{V_j}\right]\{C_i\} + \left[\frac{E_{i,j}A_j}{\ell_{i,j}V_j}\right]\{C_i - C_j\} \qquad (17)$$

where i = subscript denoting adjacent compartments

j = subscript denoting the j^{th} compartment

C_j = total pesticide concentration in a compartment ($\mu g/\ell$)

C_i = total pesticide concentration in an adjacent compartment ($\mu g/\ell$)

$Q_{i,j}$ = flow into compartment j (m^3/d)

$Q_{j,i}$ = flow out of compartment j (m^3/d)

$f_{1,j}$ = dissolved fraction of a pesticide in compartment j

$f_{2,j}$ = particulate fraction of a pesticide in compartment j

K_{da} = sum of dissolved reaction rate constant (d^{-1})

K_{pa} = sum of particulate reaction rate constant (d^{-1})

$k_{s,i}$ = settling rate constant for compartment j (d^{-1})

$k_{s,j}$ = settling rate constant from an above compartment (d^{-1})

$E_{i,j}$ = bulk dispersion coefficient between adjacent compartments (m^2/d)

A_j = surface area of compartment j (m^2)

$\ell_{i,j}$ = length between the midpoints of adjacent compartments (m)

V_j = compartment volume (m^3)

V_i = volume of adjacent compartment (m^3)

The equations comprise a set of linear, ordinary differential equations which were numerically integrated via a fourth order Runge-Kutta approximation technique.

RESULTS AND DISCUSSION

Fate and Transport

The first step in fate and transport modeling is to determine the predominant reaction and transport pathways. Coralville is a short detention time, flood control reservoir with a mean annual hydraulic detention time of only 14 days. This corresponds to a washout rate of 0.0714 day^{-1} or approximately 7% of the dissolved material is exported through the outflow on an average day. Washout is expected to be a major transport mechanism in Coralville Reservoir. Other reaction rates and partition coefficients have been measured in laboratory studies and are summarized by pollutant in Tab. I-2 Dieldrin should strongly adsorb to sediments and bioconcentrate, but degradation reactions are very slow. Furadan^R, a carbamate insecticide, is quite reactive, but biological degradation should predominate (Tab. I-2). Selected herbicides and insecticides of usage in Iowa are listed in Tab. I-2 with their laboratory protocol rate constant, half-lives, and partition coefficients.

The dieldrin time series of Fig. I-4 (dashed line) is from monthly grab sample data collected by The University of Iowa Hygienic Laboratory and indicates a steady decline in the envelope of peak concentrations during agricultural runoff events, as well as a decline in average annual concentrations. It is believed that the decline in dieldrin from the Reservoir outlet is due to the decreased aldrin application rates since 1967 as well as the microbial degradation of dieldrin by soil organisms on the land. Dieldrin loading rates in a small watershed runoff study from 1974 have been computed and range from 1.0×10^{-11} to 1.0×10^{-9} kg/m^2 - day, depending on the streamflow and hydrograph [19].

Two Compartment Model

The goal of this simulation was to analyze annual average concentrations, so transport properties (i.e., flow, volume, and sedimentation rate) were averaged over the period of simulation. A two compartment model as depicted in Fig. I-2 was utilized. Preliminary model results are presented for the Coralville Reservoir outflow in Fig. I-4. The dashed line in Fig. I-4 represents monthly grab sample field measurements, and the solid line is the annual average model simulation. Note the smooth decline in total and dissolved dieldrin concentrations due to an exponentially decreasing input loading function (Fig. I-5). The peak concentrations during runoff events recorded in the field data are not matched by the model results, since average inflow and a smooth loading rate function was assumed.

A sedimentation coefficient (k_s) of 0.18 per day was calculated from suspended solids removal rates in the Reservoir while a partition coefficient of 6250 µg/kg per µg/l (Kp) was estimated from field data [6]. The average suspended solids (M) in the reservior from 1968-78 was 80 mg/l, so KpM was 0.50, indicating the ratio between the particulate and dissolved pesticide. Initially the total pesticide inflow concentration was 0.05 µg/l, but it was assumed to decline exponentially thereafter. The sum of the first order and pseudo-first order rate constants for dieldrin are believed to be quite small. The sum of the volatilization, biolysis, photolysis, and hydrolysis rate constants was assumed to be 1.7×10^{-4} per day or a half life of 11 years. At this rate, the decay reactions were insignificant compared to the transport and sedimentation of dieldrin. The pesticide is acting as an adsorbing, conservative substance and is tracking the input loading function of Fig. I-5.

Fig. I-6 presents the mass flux of particulate adsorbed dieldrin to the bottom. Solids were assumed to be permanently lost from the water column, so the model fails to include scour. Alternatively one could consider k_s to be an "apparent" or "effective" sedimentation coefficient, the net result of sedimentation minus scour. The mass transport to the sediments involves small quantities of pesticides, from 0.068 kg/day in 1968 to less than 0.014 kg/day in 1978, or about 46 percent of the total dieldrin input. The rate of decline in dieldrin transport to the sediment parallels, and is driven by, the declining input function. Sixty-four percent of the total dieldrin in the inflow to the reservoir model was in the particulate phase (KpM = 1.79). For a solids trap efficiency of 72% [20], a corresponding dieldrin removal of 46% was indicated.

A sensitivity analysis was performed in order to assess the importance of the partition coefficient and is presented in Fig. I-7. Fig. I-7 indicates that a several fold increase or decrease of KpM from 0.50 to 2.0 or 0.10, changes the total concentration by -47 and +49 percent, respectively. The particulate fraction in Coralville Reservoir is only 33 percent of the total dieldrin if KpM is 0.50 (0.33 = (KpM)/(1+KpM)). Kellogg and Bulkley [1] indicated the same average in weekly samples from the Des Moines River, Iowa, during 1973.

The sedimentation coefficient (k_s) also affects the dieldrin removal by sedimentation. Fig. I-8 indicates that an increase of the coefficient from 0.18 to 0.28 per day results in a decrease of total dieldrin of 30 percent. The mass flux of dieldrin to the sediment (k_sC_pV) does not fully double when the sedimentation coefficient doubles due to a decreased particulate concentration in the reservoir, C_p. This sedimentation coefficient corresponds to a settling velocity of k_s times the mean reservoir depth, or 0.44 m/day. The geometric mean diameter of a particle which settles at 0.44 m/day is about 3 µm, the fine silt/clay size range. Although size distributions have not been determined for particles within Coralville Reservoir, the mean particle size of the inflow is approximately 15 µm, a silt size classification. It is expected that the mean particle size of the inflow should be greater than the mean size within the Reservoir.

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Results presented in Figs. I-4-8 did not include biological uptake by fish. Fig. I-9 is identical to Fig. I-4 except for including the effects of biological uptake and metabolism. Fish biomass and productivity in Coralville Reservoir is extremely large, estimated at 1,000 lb/acre (0.11 kg/m^2) (46 mg wet weight per liter at conservation pool). Although the fish biomass is large, the decrease in total dieldrin concentration due to uptake by fish was less than 0.002 μg/l after 10 years of simulation. This fact is attributed to the rapid rates of pesticide washout and sedimentation in Coralville Reservoir.

Fig. I-9 presents the model results and field data for dieldrin residues in sediment and the edible tissue of bottom feeding fish in Coralville Reservoir. Fish taxa include bigmouth buffalo, carp, carpsucker, catfish, and channel catfish. Fish were collected by shocking and were subsequently filleted and analyzed [21, 22, 23]. Model coefficients included:

$k_1 = 0.027/\text{day}$	uptake rate constant
$k_d = 0.0083/\text{day}$	depuration rate constant
$B = 4.67 \times 10^{-5}$ kg/l	biomass concentration
$F_o = 1150$ μg/kg	initial whole body residue
$k_2 = 0.005/\text{day}$	sediment biological degradation

A total of 1.4 percent per day of the dissolved pesticide is filtered by bottom feeding fish. The rate constants are in relative agreement with those of Thomann [24]. The effective fish filtration rate was 600 liters filtered per kg of wet fish per day and was utilized in the estimation of k_1. The partition coefficient between fish and water was estimated from field data to be 70,000 μg/kg per μg/l. Note that this is more than ten times the equilibrium partition coefficient for dieldrin between suspended solids and water. Dieldrin concentrates in bottom feeding fish due to large uptake and relatively small depuration rates.

The sediment compartment receives the mass flux of dieldrin depicted in Fig. I-6 due to sedimentation. The mass of dieldrin in the sediment is strongly partitioned into the particulate phase by adsorption. The ratio of particulate dieldrin to dissolved dieldrin is equal to KpM or approximately 2,000, assuming a solids concentration in the sediment of 0.32 kg/ℓ. The decline in sediment concentration follows the declining mass input rate to the sediment (Fig. I-6), but it also biodegrades at a rather slow rate of ∿0.005 per day. Biodegradation in the sediment compartment is assumed to occur for both dissolved and particulate dieldrin.

Bioconcentration of hydrophobic pesticides in Coralville Reservoir fish is directly proportional to the oil or lipid content of the catch. By normalizing all of the fish residue data on an oil basis, it is possible to use Equations 12 and 13 to simulate all taxa of fish simultaneously. The oil content is the fraction of the total wet weight which is extractable with petroleum ether. Fig. I-10 presents results for all fishes in which a measurement of oil content was performed. While the data are sparse, it appears that such a simple bioconcentration model has validity. The only difference between the simulations depicted in Figs. I-9 & 10 is the biomass (wet weight vs. oil) and the corresponding BCF factor (in fish flesh vs. oil). The uptake and depuration rates remain constant.

The results of Figs. I-9 and 10 indicate that the average catch no longer exceeds the FDA action level of 300 μg/kg residue. Uptake by fish accounts for almost 10% of the inflow dieldrin loading, while ∿42% of the inflow undergoes sedimentation to the bottom of the reservoir, and 48% is exported through the outflow. The partitioning of dieldrin in the water column is 64% in the fish, 24% dissolved in the water, and less than 12% adsorbed to suspended solids. Sediment and fish (and fish oil) are essentially in equilibrium with mean dissolved dieldrin concentrations. If biouptake is ignored in the model or if depurated dieldrin is not metabolized but rather returned to the dissolved phase, then the transport in the outflow is 54% and the net sedimentation is 46% of the total dieldrin load.

Eight Compartment Model

Results of the eight compartment model are presented in Figs. I-11 and 12. Field data were not available for each compartment. The field site of Fig. I-11 is downstream from the Reservoir at Iowa City and most closely represents the hypolimnion compartment 6 and the epilimnion compartment 3. There appears to be good agreement between model results and field observations.

The addition of compartments to the model provides insight into the dynamics of dieldrin transport, scour, and deposition. The only difference between the two compartment and the eight compartment model was that a small amount of scour was introduced into the sediment compartment, resulting in a lower net sedimentation rate. Compartmentalization of the system roughly offset this effect. Resulting dieldrin concentrations in the dissolved, particulate, and sediment phases all decreased proceeding downstream through the Reservoir, a result of sedimentation from the water column of a progressively lower particulate dieldrin concentration. A check on the mass balance of solids in the reservoir model indicated that sedimentation was greater than scour, which is also true of the prototype system. Scour of dieldrin from the sediment to the water was a small but significant contribution to the mass balance at the sediment-water interface. Bulk dispersion coefficients in the vertical and longitudinal directions were 9.3×10^{-4} and 4.6×10^{-4} m^2/d, respectively, with a dispersive scour at the sediment-water interface of 1.5×10^{-4} m^2/d.

The addition of compartments to the model is not an arbitrary choice. It should reflect the physical geometry of the prototype and/or the estimated dispersion pattern. Assuming a longitudinal dispersion coefficient of ∿4 mi^2/day, it is possible to estimate the proper number of

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longitudinal compartments necessary to reflect this degree of dispersion. For Coralville Reservoir, approximately 10 reactors in series would be required disregarding any bulk dispersion between compartments. As you increase the number of compartments, the model becomes more "plug-flow" in nature. Since a greater amount of material will settle out in a "plug flow" system, it would be necessary to decrease the sedimentation rate constant to reflect the field data.

Unsteady Flow Simulations

Errors are generated in the annual average, steady flow simulations (Figs. I-4-12). Mass fluxes are underestimated by using annual average flowrates and calibrating the model output with annual average water concentrations. For this reason an unsteady flow simulation was performed for dieldrin in Coralville Reservoir during 1976. Inflow and outflows are shown in Fig. I-13. Note that the reservoir volume was drawn-down from February - May and subsequently refilled. Input of dieldrin was unmeasured, so this calibration involved fitting the measured output dieldrin concentration by adjusting the inflow concentration (Fig. I-14). Mass flux to the sediment (Fig. I-15) is approximately 5% larger than that of the steady flow results if they are run with comparable input loadings. Such errors would be even larger for simulations with time variable loadings of suspended solids.

If the goal is to accurately reflect mass fluxes of sediment and dieldrin, then one must use a fully time variable approach. If annual average exposure concentrations are all that is required, then a steady flow approach similar to Figs. I-4-12 is warranted.

The mass flux to the sediment shown in Fig. I-15 provides information about seasonal variations that is not possible with annual average simulations. It has been observed that fish, especially bottom feeding fish, reach peak residue levels of dieldrin and other insecticides in June. This is due to higher dieldrin concentrations in the water as well as more recently contaminated sediment following spring runoff.

SUMMARY

Fate and transport of the pesticide dieldrin has been simulated in Coralville Reservoir. From the dieldrin analysis it was determined that 40% of the dieldrin inflow to Coralville Reservoir is lost to the bottom via sedimentation and 50% is released through the dam gates of this short detention time Reservoir. Uptake by fish accounts for about 10% of the dieldrin input due to the extremely large biomass of biota, 1000 lb/acre. The partitioning of dieldrin in the water column is 64% in the fish, 24% dissolved in the water, and less than 12% adsorbed to suspended solids. Mean residues in the edible tissue of bottom feeding fish declined below the FDA guideline of 300 ppb. Fish and sediment concentrations are essentially in equilibrium with mean dissolved dieldrin concentrations. Under low flow conditions, the sediment becomes a net source for pesticide in the Reservoir via desorption and pore water diffusion.

It was determined that bottom feeding fish bioaccumulate dieldrin in proportion to the oil content (petroleum ether extraction) of the fish sample. Therefore averages or composites of very oily fish tended to be higher than model predictions. The prospect for a continued decline in dieldrin residues is good. Model projections indicate that by 1986, the residues in bottom feeding fish flesh should average less than 100 μg/kg. Research follows in the next chapter on the role of sediment water interactions and food items on the bioaccumulation potential of the fishery.

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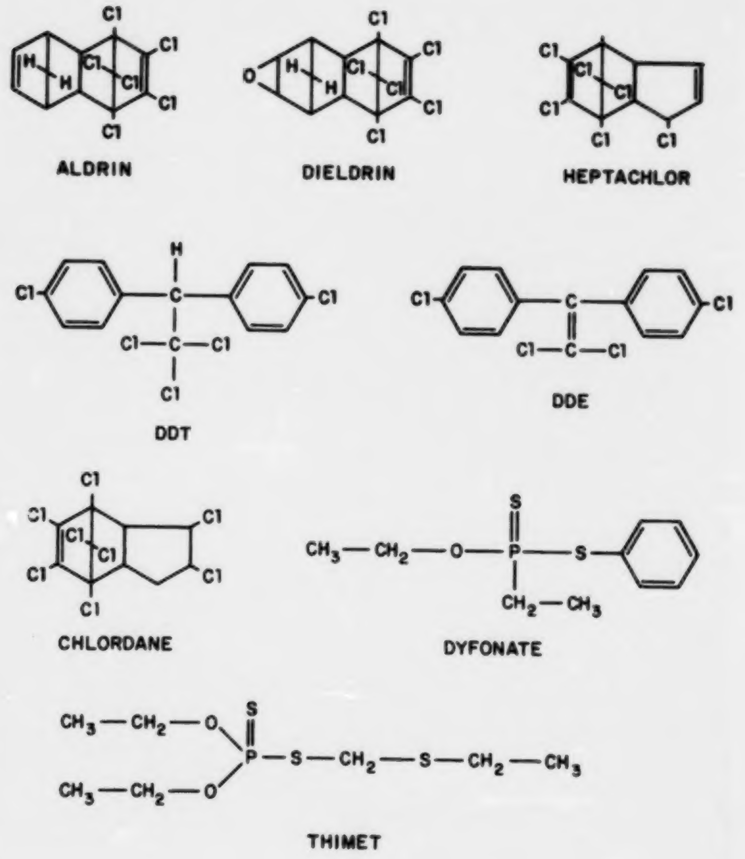
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DYFONATE
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Table I-1. Chemical Structures of Selected Iowa Pesticides

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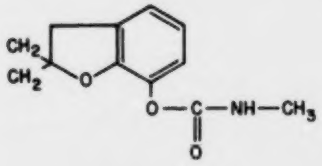

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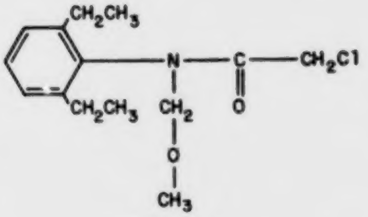

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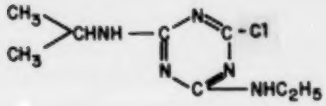

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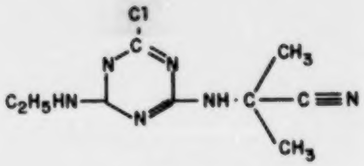

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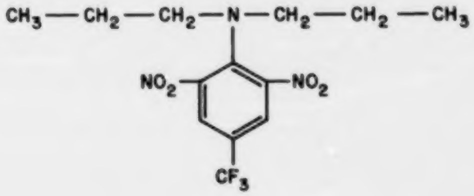

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TABLE I-2. PHOTOLYSIS, HYDROLYSIS, BIOLYSIS, AND SORPTION COEFFICIENTS FOR SELECTED IOWA PESTICIDES

	Near Surface Direct Photolysis		Alkaline Chemical Hydrolysis		Biolysis		Sediment/H_2O Partition Coeff.	Fish/H_2O Bioconcentration
	k_p, day^{-1}	$t_{1/2}$, days	k_B, $M^{-1}sec^{-1}$	$t_{1/2}$, days	$\frac{\hat{\mu}}{YK_M}$ $\left(\frac{org\text{-}hr}{l}\right)^{-1}$	$t_{1/2}$, days	$\frac{\mu g/kg\ dry}{\mu g/l}$	$\frac{\mu g/kg\ wet}{\mu g/l}$
Dieldrin	†	†			†	>10,000	10,000	10-100,000
DDT	†	†			†	†	100,000	130,000
DDE	0.7	1 [9]	~10^{-3}	1000 [10]	†	†	100,000	70,000
Furadan	0.003	~200 [11]	6×10^{-5}	>10,000 [11]	~10^{-11}	~3 [11]	500	10
Dyfonate, Thimet, Counter	†	†	10^{-4}	>365	4×10^{-10}	~9 [12]	200-500	
Atrazine	9×10^{-6}	81,000	10^{-16}	742 [13]	~10^{-11}	35	5-30	80
Cyanazine				>365	~10^{-11}	35	3-30	30
Lasso				>365	~3×10^{-11}	12	50	~75
Treflan	0.03	22 [14]			†	†	500	1800-5800 [15]

†Denotes probable reaction of unknown rate

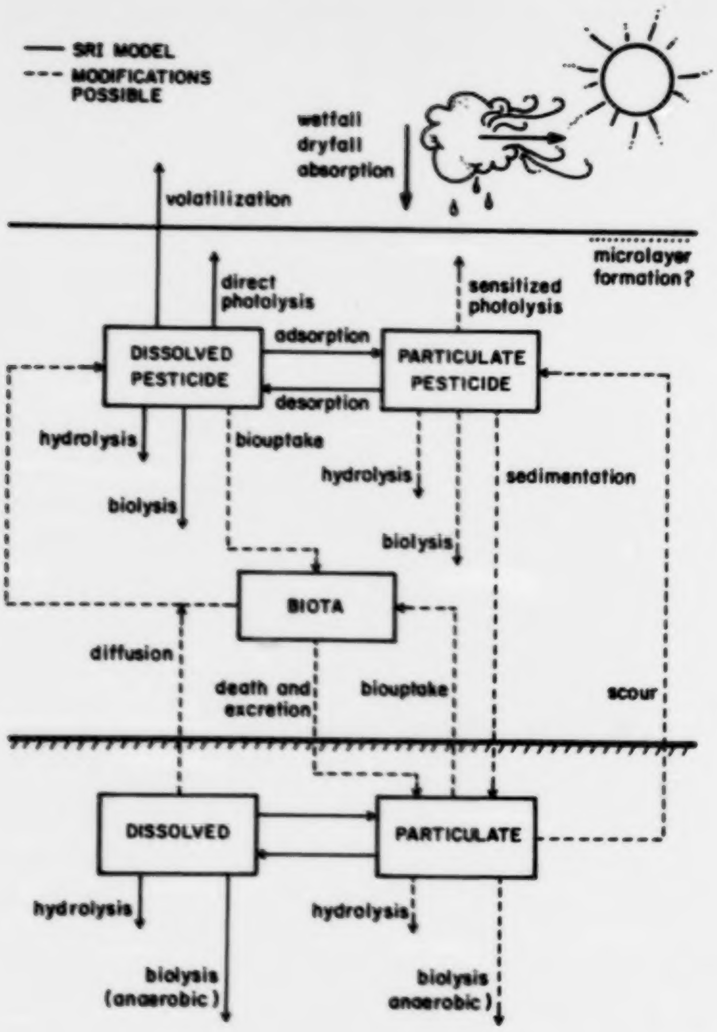
SRI MODEL
MODIFICATIONS POSSIBLE
wetfall
dryfall
absorption
volatilization
microlayer formation?
direct photolysis
sensitized photolysis
adsorption
desorption
DISSOLVED PESTICIDE
PARTICULATE PESTICIDE
hydrolysis
biouptake
biolysis
hydrolysis
sedimentation
biolysis
BIOTA
diffusion
death and excretion
biouptake
scour
DISSOLVED
PARTICULATE
hydrolysis
hydrolysis
biolysis (anaerobic)
biolysis anaerobic)

Figure I-1. Pesticide Fate and Transport

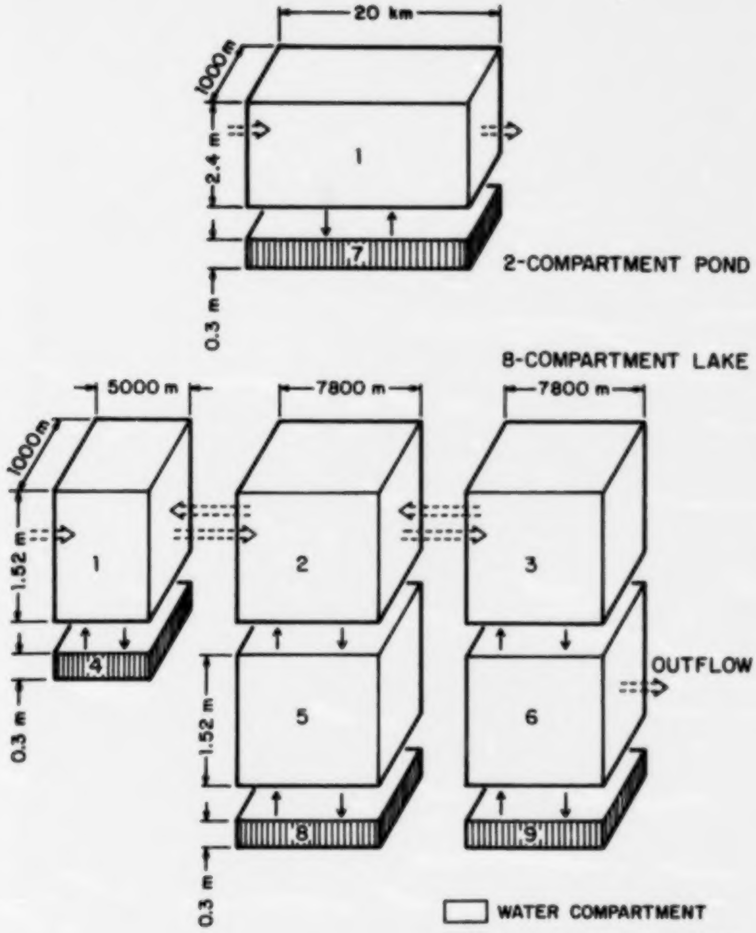
20 km
1000m
2.4 m
1
7
0.3 m
2-COMPARTMENT POND
8-COMPARTMENT LAKE
5000 m
7800 m
7800 m
1000m
1.52 m
1
2
3
4
0.3 m
1.52 m
5
6
OUTFLOW
8
9
0.3 m
WATER COMPARTMENT
SEDIMENT COMPARTMENT

Figure I-2. Physical Configurations of the Reservoir Model

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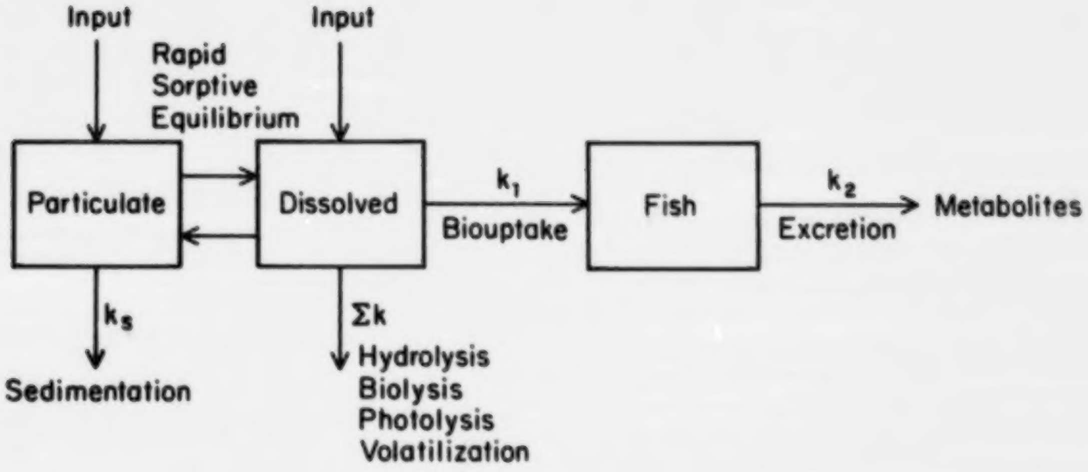
Input
Rapid Sorptive Equilibrium
Input
Particulate
Dissolved
k_1
Biouptake
Fish
k_2
Excretion
Metabolites
k_s
Sedimentation
Σk
Hydrolysis
Biolysis
Photolysis
Volatilization

Figure I-3. Bioaccumulation Kinetics of the Pesticide Transport Model

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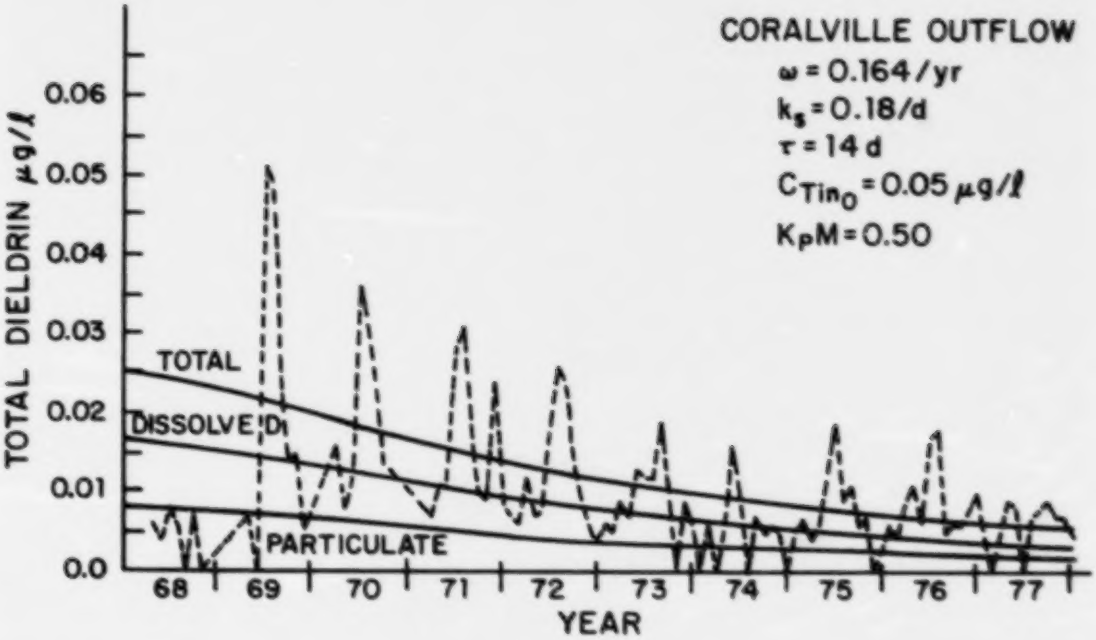

Figure I-4. Model Results for Dieldrin Concentration in the Coralville Reservoir Outflow

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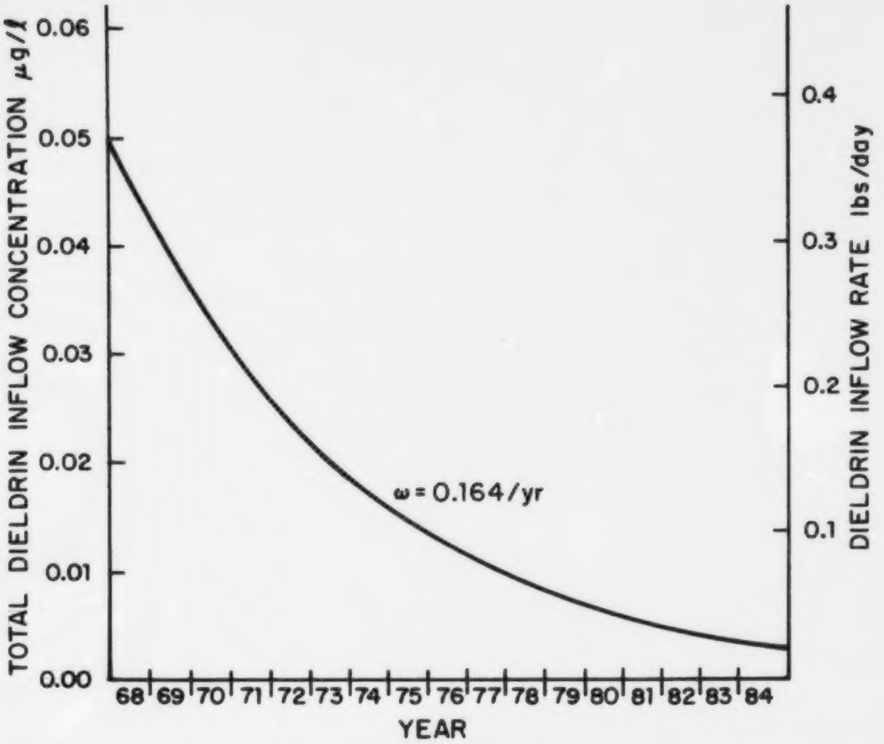

Figure I-5. Input Loading Function to Coralville Reservoir

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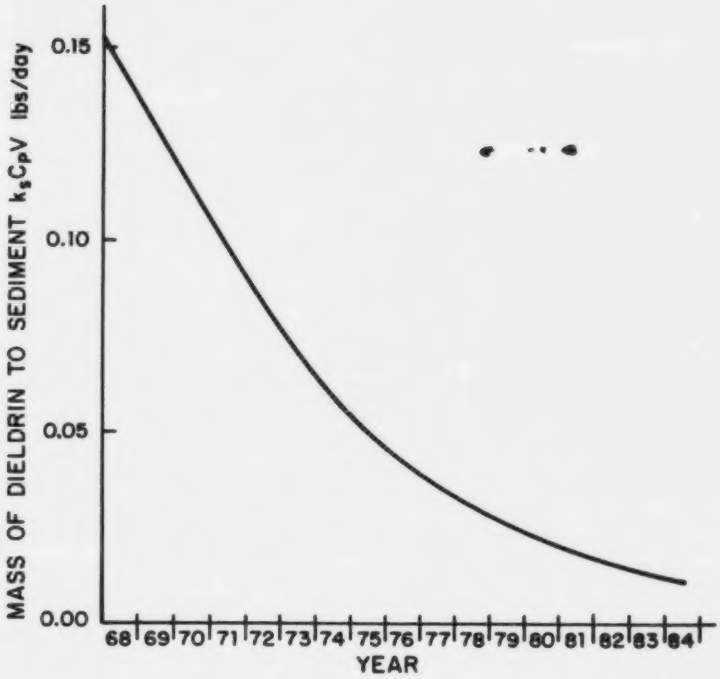

Figure I-6. Calculated Mass Flux of Dieldrin to the Sediment

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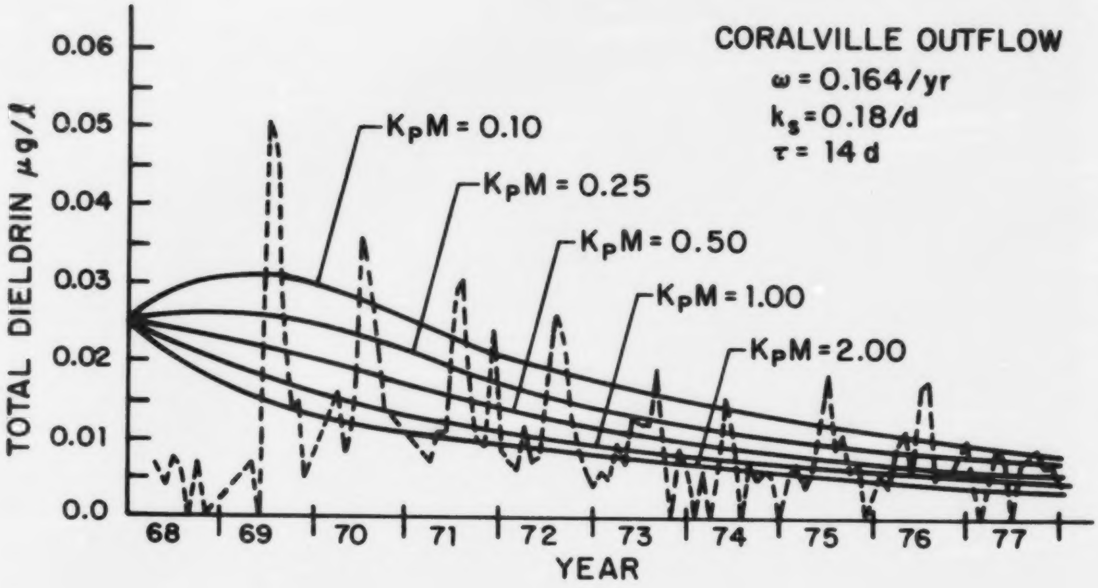

Figure I-7. Sensitivity Analysis of the Effects of the Partition Coefficient, K_p

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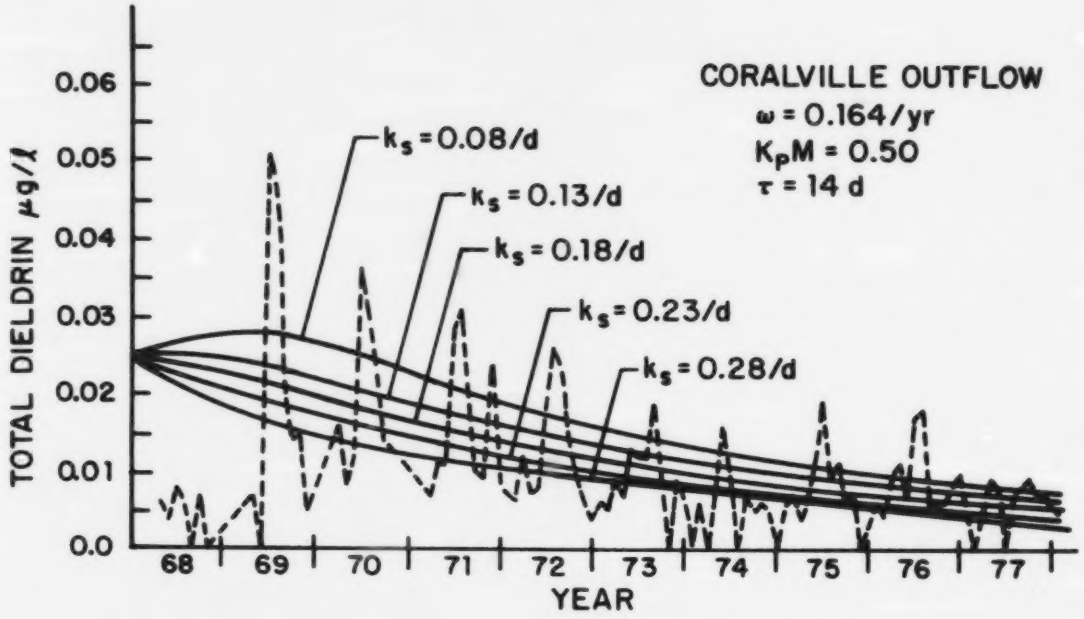

Figure I-8. Sensitivity Analysis of the Effect of the Sedimentation Coefficient, K_s

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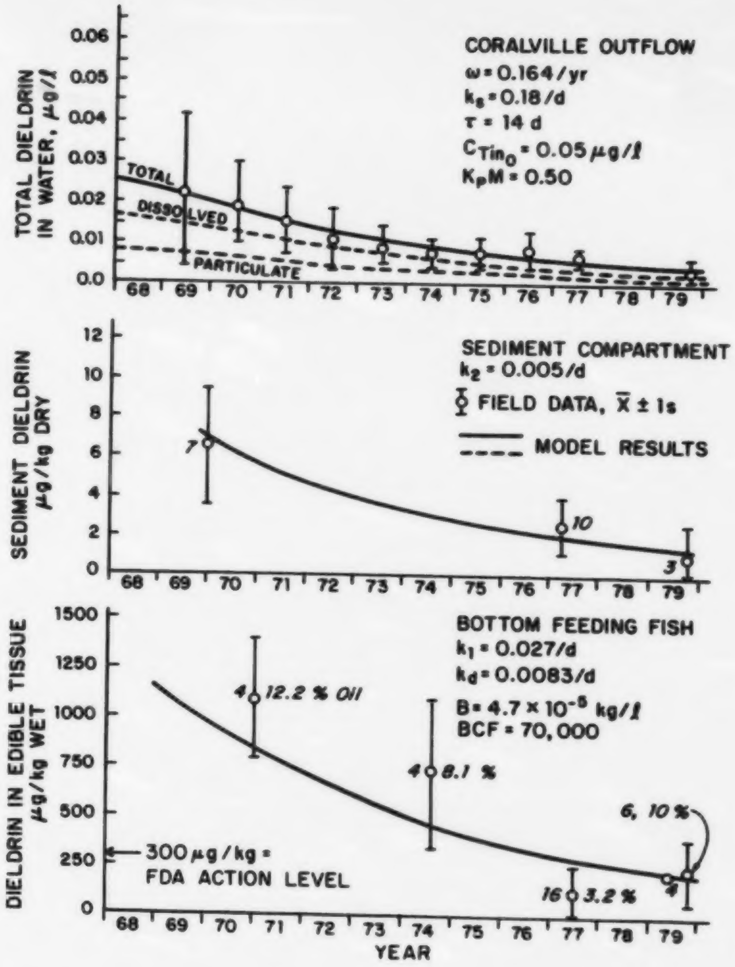

Figure I-9. Field Data and Model Results for Dieldrin in Coralville Reservoir. Numbers represent the number of data points and percentages are the percent oil or lipid content of the catch.

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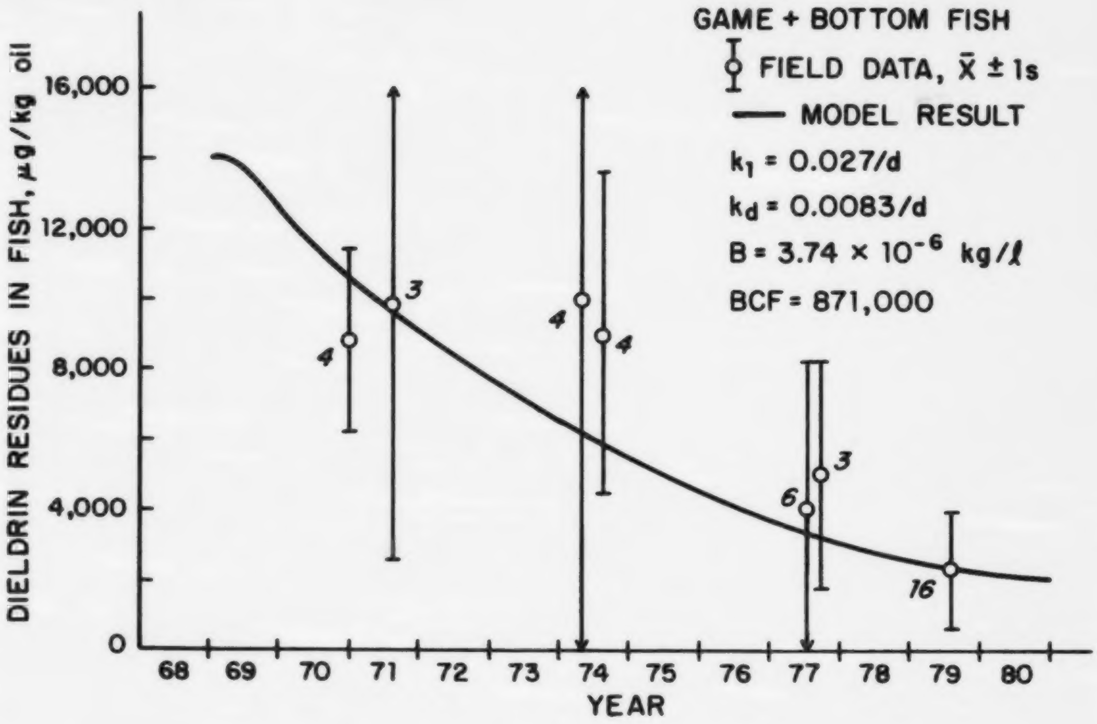

Figure I-10. Field Data and Model Results for Dieldrin in Coralville Reservoir Fish, Normalized on an Oil Basis.

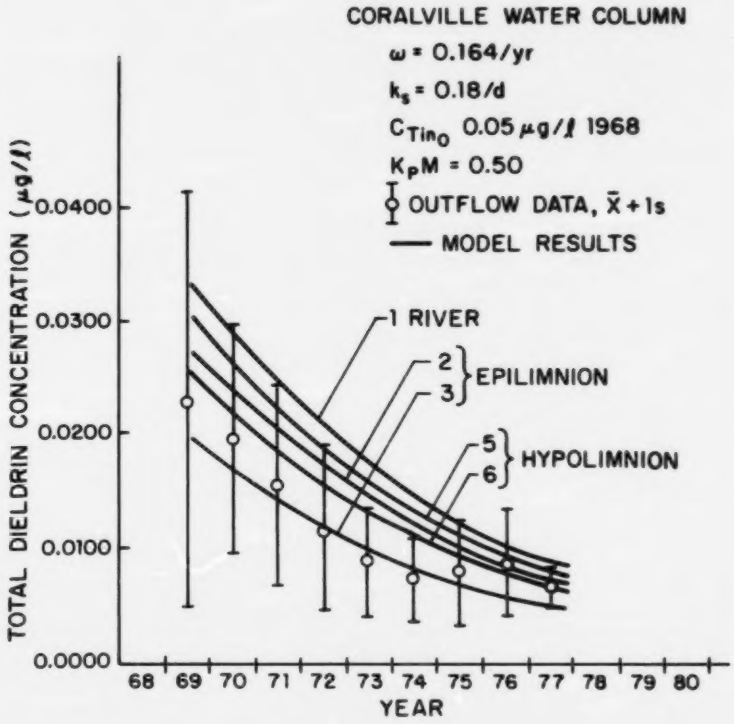

Figure I-11. Eight Compartment Model Results for Dieldrin in the Water Column.

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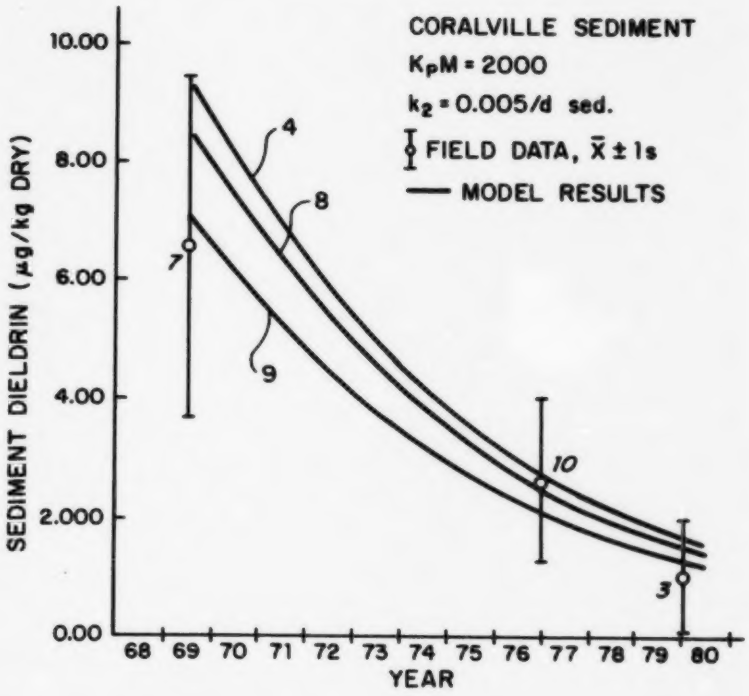

Figure I-12. Eight Compartment Model Results for Adsorbed Dieldrin on the Sediment

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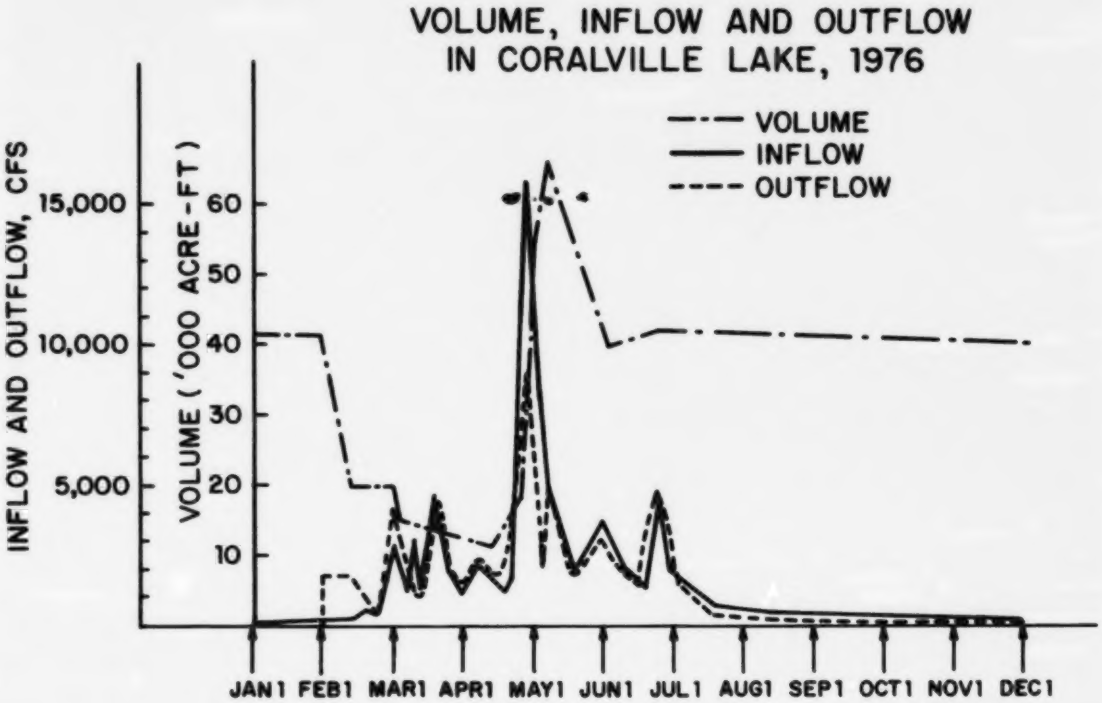

Figure I-13. Input Data for Unsteady Flow Simulation

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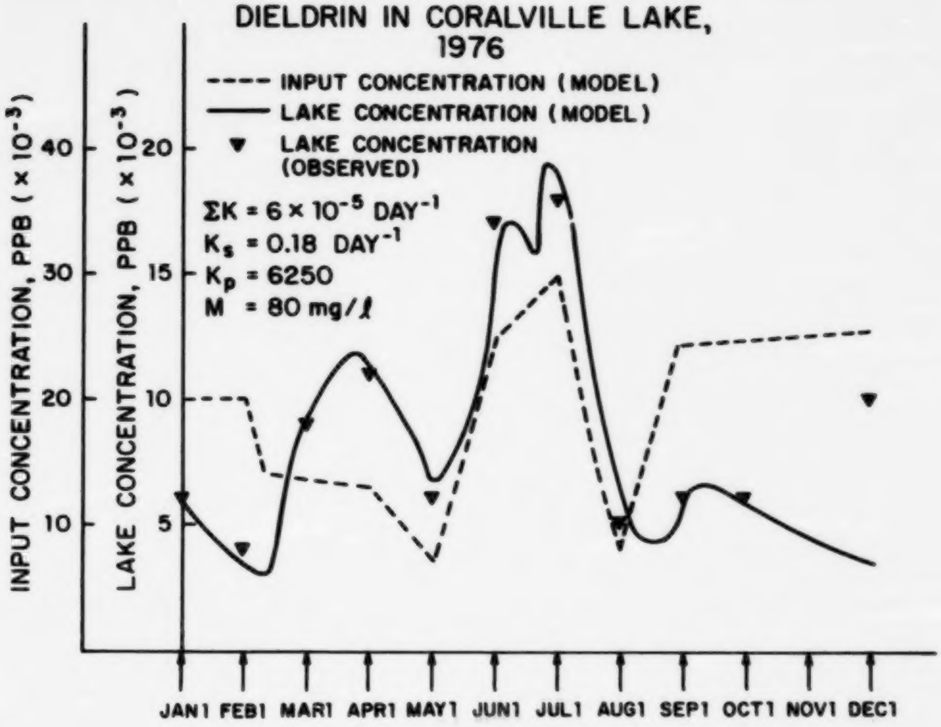

Figure I-14. Model Results for Unsteady Flow

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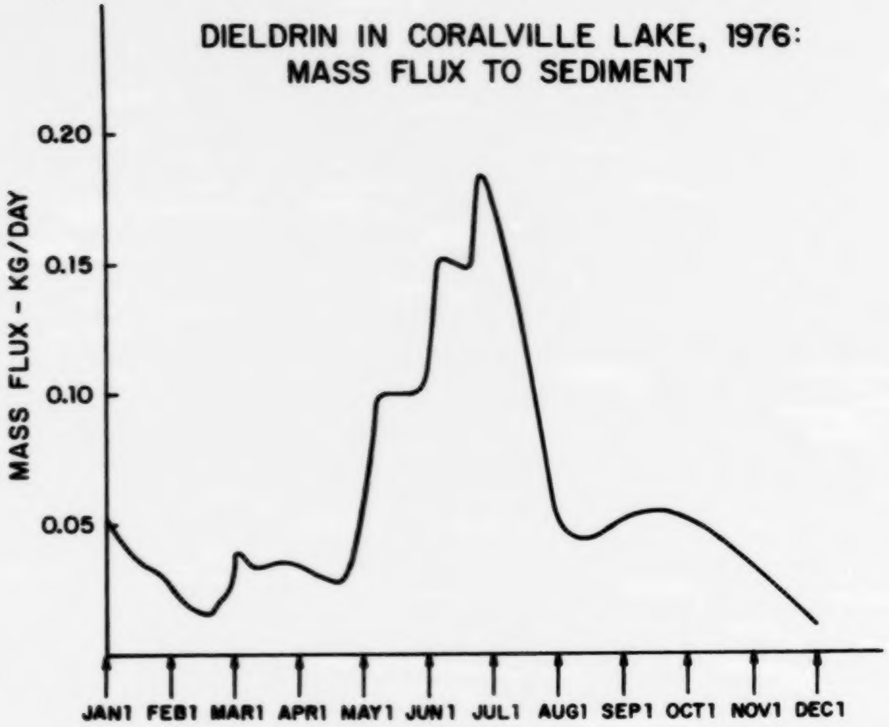

Figure I-15. Unsteady Mass Flux to the Sediment

CHAPTER II

SEDIMENT, WATER AND BIOTA INTERACTIONS OF THE PESTICIDE DIELDRIN IN CORALVILLE RESERVOIR

INTRODUCTION

Dieldrin inputs to Coralville Reservoir emanated as nonpoint source runoff after the application and microbial epoxidation of the insecticide aldrin. Aldrin and dieldrin were banned by the U.S. Environmental Protection Agency (EPA) in 1975. As applications of aldrin decreased between 1965 and 1975 due to insect resistance, there was a corresponding decrease in total dieldrin in water samples(Fig. II-1). Peak dieldrin concentrations in the water column generally correlated with high flows and turbidity (suspended solids).

A hypothetical scenario for the "self-purification" of an impoundment after pollution by a hydrophobic, persistent. toxic organic is depicted in Fig. II-2. As with dieldrin in Fig. II-1, the concentration of toxin in the water column decreases after the discharge decreases. For a period, fish bioconcentrate the toxic from the dissolved phase -- they "track" the water column with a slight time lag on the order of a few weeks to a few months. The rate of sediment contamination depends on the rate of deposition of suspended solids and the mixing characteristics of sediment and water. As the water column concentration and fish residues decline, there is a period when the fish body burden is taken predominantly from sediment ingestion and other food items. This occurs due to the low concentration in the water and lagging sediment and biota residue levels.

Finally even the sediment declines in concentration due to desorption - diffusion into the water column and due to sediment burial and mixing. It is the last phase of the scenario of Fig. II-2 that best describes the current situation in Coralville Reservoir for dieldrin, chlordane, DDE, and heptachlor epoxides. All of these chemicals have been banned, yet all of them continue to bioaccumulate to objectionable levels in fish despite water concentrations below detection limits in most cases. One of the chemicals, DDE, is apparently generated by dehydrochlorination in sediment and is slow to decline. A more detailed analysis of the dieldrin field data in Coralville Reservoir provides evidence of the importance of sediment-water-biota interactions.

FIELD OBSERVATIONS

Dieldrin is declining in the Coralville Reservoir outflow. Both the annual average concentration, the annual maximum concentration, and the coefficient of variation have declined since 1969 (Tab. II-1). From 1965-1975, peak concentrations occurred after spring application and runoff. Presently the peak annual dieldrin concentration is much smaller ($\sim$0.010 μg/ℓ) and can occur any time throughout the year. Often peak concentrations are still associated with high flows, but "background" concentrations and baseflow concentrations are nearly as large as the annual peak. The reservoir system is being "buffered" by inputs from the sediments during moderate flow and low flow conditions.

Suspended solids in the outflow from Coralville Reservoir correlate strongly with flow, as can be determined from the time series of Fig. II-3 This is due to higher shear stress near the bottom of the Reservoir during high flows and due to increased sediment carrying capacity. Partheniades [1] showed the relationship between average bottom shear stress and rate of erosion of bed sediment (Fig. II-4). Unfortunately the power of the relationship of Fig. II-4 (n = 1 to n = 3) has been shown to vary widely among various cohesive sediments and investigators. It is virtually impossible to predict the rate of scour *a priori* without very detailed knowledge of the cohesive sediment properties (e.g. tensile strength, plasticity index, clay content, compacted density, etc.)

Because of scour and resuspension of bed sediment, bank erosion, and increased sediment carrying capacity, dieldrin loading and suspended solids loadings are highly correlated as shown in Fig. II-5. It is interesting to note that during the 100-year drought of 1976-1977, stream flows carried negligible solids, but the dieldrin loading was nevertheless significant (Fig. II-5). This is even more evident in Fig. II-6, showing the relationship between suspended solids loads and total dieldrin concentration. During the drought years, 1976-77, the dieldrin concentration was quite significant. It was predominantly dissolved dieldrin from sediment desorption and dissolution. This illustrates the buffering effect that sediments can have on the water column years after the primary source of dieldrin was curtailed. While it does not amount to a large mass of dieldrin, it is a significant exposure concentration for fish bioconcentration.

Sediments are historically contaminated with dieldrin, but the degree of contamination has decreased since the ban in 1975. A typical upstream sediment core is shown in Figs. II-7 and II-8.

In sandy substrates, such as the inflow delta, finer material is deposited near the surface of the sediment under low flow, ice-covered conditions. This fine silt is characterized by high organic content and volatile solids greater than 10%. In these locations one observes a maximum dieldrin concentration in surficial sediments(Fig. II-8a). The bed is continuously being reworked each year, and the fine silts will be subsequently scoured, resuspended, and deposited downstream. An interesting feature of Fig. II-8b is the relatively constant sediment concentration with depth on a volatile solids basis. There are some indications that the sediment is disturbed enough to create rather uniform concentration profiles on a volatile solids basis. This could indicate thermodynamic equilibrium is achieved in mixed sediments.

The site of Figs. II-7 and 8 is characterized as one of intermediate deposition located near the inflow to Coralville Reservoir. Bed surfaces would be subject to scour and resuspension. A low density of nematodes and _Chironomid_ _sp_. were observed in the core samples. However bioturbation of these areas is expected primarily by carp and other bottom feeding fish which are in abundance. Carp, carpsucker, red horse, and buffalo are known to work the sediments in this area. Model results indicate that bioturbation of this sort can serve to increase the sediment flux of contaminants by several fold.

A point in contrast is the sediment concentration profiles in highly depositing basins of the reservoir. In Coralville Reservoir, the annual average deposition is 5.8 cm/year. In deep, highly depositional zones, the high rate of sedimentation of cohesive sediments precludes a great degree of mixing. Field data, although it is sparse, supports the conclusion that some degradation of dieldrin is occurring in the sediment -- otherwise sediment concentration profiles would be considerably larger. Interstitial waters track the sediment concentration very well. Diffusion and sorption of dissolved dieldrin to the sediment from the water column may occur if sediment degradation reactions decrease sediment and interstitial concentrations as shown. Otherwise the sediments serve as a source of dieldrin to the water column by scour/resuspension, and desorption/diffusion.

MODELING SEDIMENT-WATER INTERACTIONS

Compartmentalization

The model of Schnoor [2] and Schnoor and McAvoy [3] was further developed to include a variable sediment volume (sediment burial) and was extended to 25 compartments. Fig. II-9 is a schematic of the compartmentalization.

The average longitudinal dispersion coefficient in Coralville Reservoir was estimated from the formula by Liu [4] to be approximately 4 mi^2/day. Twenty-five compartments would yield a numerical dispersion of this same magnitude according to Equation 18:

$$E_x = \frac{u\Delta x}{2}\left(1 - \frac{u\Delta t}{\Delta x}\right) \qquad (18)$$

where E_x = longitudinal dispersion coefficient, L^2/T

u = mean velocity, L/T

Δx = compartment length, L

Δt = time step, T

Therefore, no bulk longitudinal dispersion was required in the model since compartment volumes were chosen such that the artificial dispersion would approximate the in-situ estimated dispersion.

Solids Balance

Vertical bulk dispersion was required to scour and resuspend solids from the soil compartment to the hypolimnion and epilimnion compartments. The vertical dispersion coefficient ($E_Z = 1.0 \times 10^{-4}$ m^2/day) and the suspended solids sedimentation rate constant ($k_s = 0.4$/day) were determined from a solids balance that was performed prior to the dieldrin simulations using the program TOXIC. The Appendix provides the user documentation for TOXIC. (Note: it is possible to perform the mass balance on suspended solids and sediment using the model TOXIC by assigning a high partition coefficient ($K_p \sim 1{,}000{,}000$) and zero degradation rate ($\Sigma k = 0$). Thus it is possible to determine the appropriate suspended solids concentrations, sedimentation rate constants, and vertical dispersion rates provided that one knows the total sediment loadings and net deposition rates or trap efficiency.) It is imperative to have accurate knowledge of the solids mass balance in order to simulate a hydrophobic toxic, e.g. dieldrin. Mass must be conserved.

The solids balance for the simulations in Chapter I utilized a bi-weekly average inflow concentration of suspended solids of 241 $\mu g/\ell$, a trap efficiency of 72%, and consequently an outflow concentration of 79 $\mu g/\ell$. The required sedimentation rate constant was determined from the solids balance to be 0.18/day.

The capacity of Coralville Reservoir was resurveyed in 1958, 1967, and 1975. From the most recent sediment survey data and from daily, flow-weighted suspended solids loadings at the inflow to Coralville Reservoir (at Marengo, Iowa), it was determined that the true solids trapped were $\sim 4 \times 10^6$ kg/day with an average annual inflow concentration of 1920 mg/ℓ. Large errors can result in the mass flux of both solids and toxics if loadings are averaged from infrequent measurements.

The modeling application here is quasi-dynamic -- the approach utilizes: 1) steady, annual average flow (from daily measurements) for long-term simulations, 2) steady, annual average, flow-weighted solids (from daily suspended solids measurements), and 3) time-variable toxicant loadings. Researchers must choose whether to simulate annual average concentrations of solids and toxics (to assess biological exposure) or whether to simulate accurately the mass fluxes to the sediment and outflow. If it is important to know both the mass flux and the exposure concentration accurately, then one should use a fully time variable model with daily (or more frequent) inputs.

In addition to utilizing the model TOXIC for solids balances, a series of simple interactive programs were developed for performing solids balances in two-compartment (sediment and water) reservoirs:

1) TWOCOMP - a constant volume compartment model for solids which interactively calls for desired simulation time, input suspended solids concentration, sedimentation concentration, and a vertical bulk dispersion coefficient

2) TWOCOMP1 - a variable volume compartment model for solids which interactively calls for the above information plus the "volume increase factor" of the aggrading sediment comparmtent (a volume increase factor of 2 will double the sediment volume linearly during the duration of the simulation)

3) PEST1 - a two-compartment pesticide model which utilizes the suspended solids concentrations generated by the model TWOCOMP or TWOCOMP1

Examples of these models appear in the Appendix.

Pesticide Balance

The final results for the PEST1 or TOXIC two-compartment model are presented in Tab. II-2. In this simulation, the volume of the sediment compartment increased at an annual rate of 5.8 cm/yr, the average rate computed from the sediment resurvey of Coralville Reservoir by the U.S. Army Engineers, Rock Island District. Results presented in Tab. II-2 are quite similar to previous results of the eight compartment model from Chapter I. Model results of Tab. II-2 are in general agreement with field observations except for the sediment residue levels (μg/kg) which are low by a factor of 2-4. This is easily corrected if we decrease the rate of degradation in the sediment to $\Sigma k = 0.0026$/day. Since the rates of degradation of sorbed toxics are often uncertain, Σk becomes a sensitive parameter about which more needs to be known.

Tab. II-3 details the results of the 25 compartment model with a sediment degradation of $\Sigma k = 0.0026$/day and a three-fold larger inflow concentration than used in Tab. II-2. The larger dieldrin loading was used as an annual average mass flux into the reservoir consistent with the updated solids balance. Results of Tab. II-3 comprise the best estimate of what has actually taken place in Coralville Reservoir on a mass flux basis.

To be certain, there are diminishing returns to simulations with greater and greater mechanistic realism and complexity. The 25 compartment simulation of Tab. II-3 did not provide significant additional insight. However it represents the best estimate of the actual dieldrin dynamics. If a management decision required quite accurate information, a model with time variable inputs may be warranted. Model complexity should fit the user's need.

A simulation was performed to determine the relative contribution of the sediment desorption and scour to the mass of dieldrin in the water column. The present internal recycle of dieldrin from the sediments is calculated as 0.003 kg/day with external loadings from inflows of 0.023 kg/day. About 12% of the dieldrin in the water comes from the sediment. If there was a total cutoff of external loadings, the 25-compartment model indicates there would be a sharp decline in dieldrin concentrations. However if this loading curtailment was in conjunction with a drought and longer detention time, then the sediment could produce as much as 6 ng/ℓ of dieldrin for a few months and 1.2 ng/ℓ for more than 2 years after the cutoff in load. Clearly the model is consistent with the record of Fig. II-6.

Burial was simulated by increasing the volume of the sediment layer in a 20 year simulation. Another option was to continually add new sediment compartments of $\sim$6 cm depth each year to simulate the net deposition in Coralville Reservoir. This proved to be rather costly in terms of computation time since a 20 year simulation would generate a total of 200 sediment compartments. The top sediment compartment of 6 cm would serve as the "active layer" while the others would be deep sediment.

The best estimate of dieldrin in sediments of highly depositional zones is presented in Fig. II-10 using a partition coefficient of 1500. In the absence of sediment degradation reactions and vertical transport, the sediment profile resembles the dieldrin loading scenario. However there has been a vertical flux of dieldrin from the sediment to the water due to resuspension and scour and a vertical migration within the sediment due to diffusion. Furthermore degradation of adsorped dieldrin results in the two profiles for the rate constants $\Sigma k = 0.07$/year and 0.95/year (half lives of 10 years and 265 days, respectively). The profile with the large sediment degradation rate of 0.95/year (0.0026/day) most closely reflects field data. Sediment cores of 100 cm can be collected at Mahaffey Bridge in the upper portion of Coralville Reservoir. Core analyses indicate no detectable dieldrin except in surficial sediment samples. The high organic content of these cohesive, mucky samples does make extraction and recovery of dieldrin difficult.

BIOTIC UPTAKE

Bioconcentration

Fish bioconcentrate dieldrin directly from dissolved residues in the water by mass transfer at soft, epithelial tissue (gills). Also there exists a strong correlation between insecticide residue levels in fish and the percent oil or fat (petroleum ether extraction). To demonstrate that the residue level of fish is directly related to their fat content, Fig. II-11 was plotted with 1979 data for a variety of fish species and seasons. Fish samples were analyzed according to US Food and Drug Administration (FDA) procedures by the University of Iowa Hygienic Lab. Fig. II-11 demonstrates that oil content removes 60% of the variance (r^2) in fish residue samples regardless of fish species. Autumn (October-November) residues in fish are lower than summer (June and August) samples, primarily due to a difference in exposure concentrations from agricultural runoff.

The slope of the line in Fig. II-11 gives the residue concentration in fish oil at 1979 exposure levels. The annual average insecticide exposure concentrations during this period were 0.005 μg/l dieldrin, $\sim$0.002 μg/l chlordane (cis-chlordane plus trans-chlordane plus nonachlor), $\sim$0.001 μg/l DDE, and $\sim$0.001 μg/l heptachlor epoxide. Based on this residue and exposure data, the oil-normalized bioconcentration factors (BCF-oil) expressed as $\log_{10}$ BCF μg/kg oil per μg/l are 5.6, 6.0, 5.9, and 5.8 for dieldrin, chlordane, DDE, and heptachlor epoxide respectively. Fig. II-12 shows the log BCF-oil plotted for a number of insecticides in Iowa waters. Oil-normalized BCFs correlate roughly with octanol water partition coefficients.

The total storage of dieldrin in Coralville Reservoir is largely in the sediment (∿45 kg). Bottom feeding fish contain perhaps 0.5 kg while the water column contains only ∿0.2 kg and particulate suspended material ∿0.1 kg. All other elements of the ecosystem contain very little dieldrin. Apparently biomagnification is not a large problem since bottom feeding fish have the highest biomass and residue levels (Fig. II-13).

Bioaccumulation

The kinetics of bioaccumulation are shown in Fig. II-14. Fish can lose unmetabolized toxics via biliary excretion or "desorption" through the gill. One the other hand, toxic organics can undergo biotransformations and be eliminated as metabolic products. The rate constant, k_2, includes total depuration (both excretion of unmetabolized toxics, k_2', and elimination of metabolites, k_2''). Only a fraction of this elimination is returned to the water column as dissolved parent compound, designated as k_2' in Fig. II-14. (Note: $k_2 = k_2' + k_2''$).

The kinetics of bioaccumulation are presented in Equation 19:

$$\frac{dF}{dt} = ek_1C/B - k_2F + k_3r_b + k_4r_f + k_5r_w \qquad (19)$$

in which

e = efficiency of toxic absorption at the gill

k_1 = biouptake rate from the dissolved phase

$$= \left(\frac{\ell \text{ filtered}}{\text{kg fish-day}}\right) \times \left(\frac{\text{kg fish}}{\ell}\right)$$

k_2 = depuration rate constant including excretion and clearance of metabolites, day^{-1}

C = dissolved toxic organic, $\mu g/\ell$

B = fish biomass, kg/ℓ

F = fish residue (whole body), $\mu g/kg$

r_b, r_f, r_w = whole body residues in bed sediment, fish prey, and worms, respectively, $\mu g/kg$

k_3 = uptake rate of bed sediment for detrivores, day^{-1}

k_4 = uptake rate of fish predation, day^{-1}

k_5 = uptake of worms and benthos, day^{-1}

The uptake rate constant from dissolved toxicant in the water, k_1, is a product of the fish respiration rate and the biomass of fish in the system. At steady state, Equation (19) admits the following solution:

$$F = \frac{ek_1C}{k_2B} + \frac{k_3r_b}{k_2} + \frac{k_4r_f}{k_2} + \frac{k_5r_w}{k_2} \tag{20}$$

This is a good form of the equation in which to evaluate the relative contribution of each term: 1) uptake of dissolved organic through the gill, 2) uptake of bed sediment, 3) uptake of fish prey, and 4) uptake of worms and benthic organisms. Figs. II-15 and 16 give the results for dieldrin uptake by gamefish and bottom fish in Coralville Reservoir. More than 50 percent of the uptake is from the water in both cases, but game fish get their second-most contribution from prey fish and bottom feeders get theirs from sediment ingestion. Results are based on field and microcosm studies and literature values of feeding rates.

Often in the case of small fish and detritivores, the predominant path of bioaccumulation is through the gill membranes. In this case bioconcentration is described by only the first two terms of equation (20). The steady state solution is then:

$$F = \frac{ek_1C}{k_2B} \tag{21}$$

in which

$$\frac{ek_1}{k_2B} = \text{the bioconcentration factor, } \frac{\mu g/kg}{\mu g/\ell}\ .$$

Bioconcentration factors normalized on a lipid basis, are especially useful since often the kinetics of uptake and depuration are rapid compared to transport and other reactions. In Coralville Reservoir, fish were at near-equilibrium with dissolved dieldrin concentrations. The response time of the fish to a step function change in dieldrin concentration is on the order of three to ten weeks, based on field data and laboratory microcosm testing. This means that fish would respond relatively rapidly to "cleanup" of an ecosystem which had been contaminated by dieldrin.

SUMMARY

Physical, chemical and biological processes are all important in the fate and transport of dieldrin in Coralville Reservoir. A good water budget and solids balance are necessary for an accurate mass balance on pesticide.

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During high flow periods, dieldrin continues to enter the Iowa River with agricultural runoff. To a lesser extent, it is scoured from contaminated sediments. Under low flow regimes, dieldrin desorbs and diffuses from contaminated bed sediments to the water column. Thus dieldrin is decreasing in the aquatic ecosystem due to washout, burial by less contaminated sediment, and possibly by degradation reactions in the bed.

Fish bioconcentrate dissolved dieldrin and, to some extent, bioaccumulate dieldrin from sediment ingestion and prey items. Since "hot spots" of dieldrin do not exist in this case, sediment and benthos ingestion are of less importance. Fish will respond to changes in dieldrin concentrations because the kinetics of bioconcentration are relatively rapid.

REFERENCES

1. Partheniades, E., "Erosion and Deposition of Cohesive Soils," Journal of the Hydraulics Division, ASCE, Vol. 91, No. HY1, Proc. Paper 4202, Jan., 1965, pp. 105-139.

2. Schnoor, J.L., "Fate and Transport of Dieldrin in Coralville Reservoir: Residues in Fish and Water Following a Pesticide Ban," Science, Vol. 211, 20 Feb., 1981, pp. 840-842.

3. Schnoor, J.L. and McAvoy, D.C., "A Pesticide Transport and Bioconcentration Model," J. Environ. Engr. Div., ASCE, Vol. 107, No. EE6, Dec. 1981.

4. Liu, H., "Predicting Dispersion Coefficient of Streams," J. Environ. Engr. Div., ASCE, Vol. 103, No. EE1, Feb., 1977, pp. 59-69.

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Table II-1. Annual Total Dieldrin Concentration Statistics from Below Coralville Reservoir at Iowa City, 1969-1979

YEAR	MEAN CONC.	S STD. DEV. µg/ℓ	%CV COEFF. VAR.	MAX CONC. µg/ℓ	N. NO. OBS.
1969	0.022	0.019	86.4	0.052	7
1970	0.019	0.010	51.1	0.035	7
1971	0.016	0.009	56.4	0.031	9
1972	0.011	0.007	61.8	0.026	12
1973	0.009	0.005	53.8	0.020	12
1974	0.005	0.005	94.4	0.016	12
1975	0.007	0.005	66.6	0.018	12
1976	0.010	0.005	53.3	0.017	11
1977	0.005	0.003	64.5	0.009	10
1979	0.008	0.001	12.5	0.010	9

Table II-2. Two-Compartment Model Results with Aggrading Sediment, Coralville Reservoir

Parameters:	$K_pM = 0.6$	water column partitioning
	$K_pM = 3210.$	sediment partitioning
	$k_s = 0.4/\text{day}$	sedimentation rate constant
	$E_z = 0.0001\ \text{m}^2/\text{day}$	vertical dispersion
	$\Sigma k = 0.000325/\text{day}$	dissolved reactions
	$\Sigma k = 0.0052/\text{day}$	sediment reactions
	$t_o = 14$ days	detention time
	$c_{in,o} = 0.050\ \mu g/\ell$	initial inflow concentration
	$\omega = 0.164$ yr.	exponential decline

DIELDRIN RESIDUES

Time (days)	Water, C_T $\mu g/\ell$	Sediment, C_T $\mu g/\ell$	Suspended Sediment, r $\mu g/kg$	Bed Sediment, r $\mu g/kg$
0	0.0250	2.25	15.6	0.70
600	0.0131	2.91	8.18	0.91
1200	0.0100	2.27	6.25	0.71
1800	0.0076	1.74	4.77	0.54
2400	0.0058	1.33	3.64	0.41
3000	0.0044	1.01	2.78	0.32
3600	0.0034	0.77	2.12	0.24

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Table II-3. Results of 25 Compartment Simulation for Dieldrin in Coralville Reservoir

TOTAL DIELDRIN CONCENTRATION, C_T(μg/ℓ)

COMPARTMENT		day 0	day 1200	day 2400	day 3600
Water	1	0.025	0.0687	0.0401	0.0234
	2		0.0544	0.0318	0.0186
	3		0.0435	0.0255	0.0149
	4		0.0351	0.0206	0.0120
	5		0.0286	0.0169	0.00983
	6		0.0232	0.0137	0.00798
	7		0.0235	0.0139	0.00811
	8		0.0176	0.0103	0.00603
	9		0.0203	0.0120	0.00702
	10		0.0144	0.00846	0.00494
	11		0.0168	0.00908	0.00578
	12		0.0124	0.00732	0.00427
	13		0.0136	0.00807	0.00471
	14		0.0112	0.00663	0.00387
	15		0.0115	0.00681	0.00397
Sediment	16	2.25	18.2	11.1	6.48
	17		13.8	8.48	4.95
	18		10.6	6.50	3.80
	19		8.08	4.99	2.92
	20		6.23	3.85	2.26
	21		5.02	3.13	1.83
	22		4.27	2.67	1.56
	23		3.28	2.05	1.20
	24		2.44	1.52	0.893
	25		1.49	0.908	0.532

Table II-3. Results of 25 Compartment Simulation for Dieldrin in Coralville Reservoir (continued)

MASS OF DIELDRIN ON SOLIDS, r(μg/kg)

COMPARTMENT		day 0	day 1200	day 2400	day 3600
Water	1	10.2	28.0	16.4	9.56
	2	11.2	24.4	14.3	8.34
	3	12.3	21.5	12.6	7.33
	4	13.6	19.1	11.2	6.55
	5	14.9	17.1	10.0	5.86
	6	18.3	17.0	10.0	5.84
	7	15.3	14.4	8.50	4.96
	8	23.4	16.5	9.70	5.66
	9	15.6	12.6	7.49	4.37
	10	27.6	15.8	9.34	5.44
	11	17.0	11.4	6.76	3.94
	12	30.6	15.2	8.97	5.23
	13	18.8	10.2	6.08	3.55
	14	33.0	14.8	8.76	5.11
	15	24.3	11.2	6.64	3.87
Sediment	16	0.97	7.82	4.77	2.78
	17	1.15	7.10	4.35	2.54
	18	1.38	6.48	3.98	2.33
	19	1.64	5.90	3.64	2.13
	20	1.95	5.40	3.34	1.96
	21	2.09	4.66	2.90	1.70
	22	2.20	4.17	2.61	1.53
	23	2.55	3.72	2.32	1.36
	24	3.05	3.32	2.07	1.21
	25	5.09	3.37	2.06	1.20

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Table II-3. Results of 25 Compartment Simulation for Dieldrin in Coralville Reservoir (continued)

PARAMETER LIST:

$K_pM = 0.22 - 2.6$	water column partitioning
$K_pM = 660 - 3{,}450$	sediment partitioning
$K_s = 0.4$	sedimentation rate constant
$E_z = 0.0001\ m^2/day$	vertical dispersion coefficient
$E_x = 0$	longitudinal dispersion
$\Sigma k = 0.000325/day$	dissolved reactions
$\Sigma k = 0.0026/day$	sediment reactions
$t_o = 14$ days	detention time
$C_{in,o} = 0.150\ \mu g/\ell$	initial inflow concentration
$\omega = 0.164/yr$	exponential decline
$K_p = 1500$	sediment: water partition coefficient

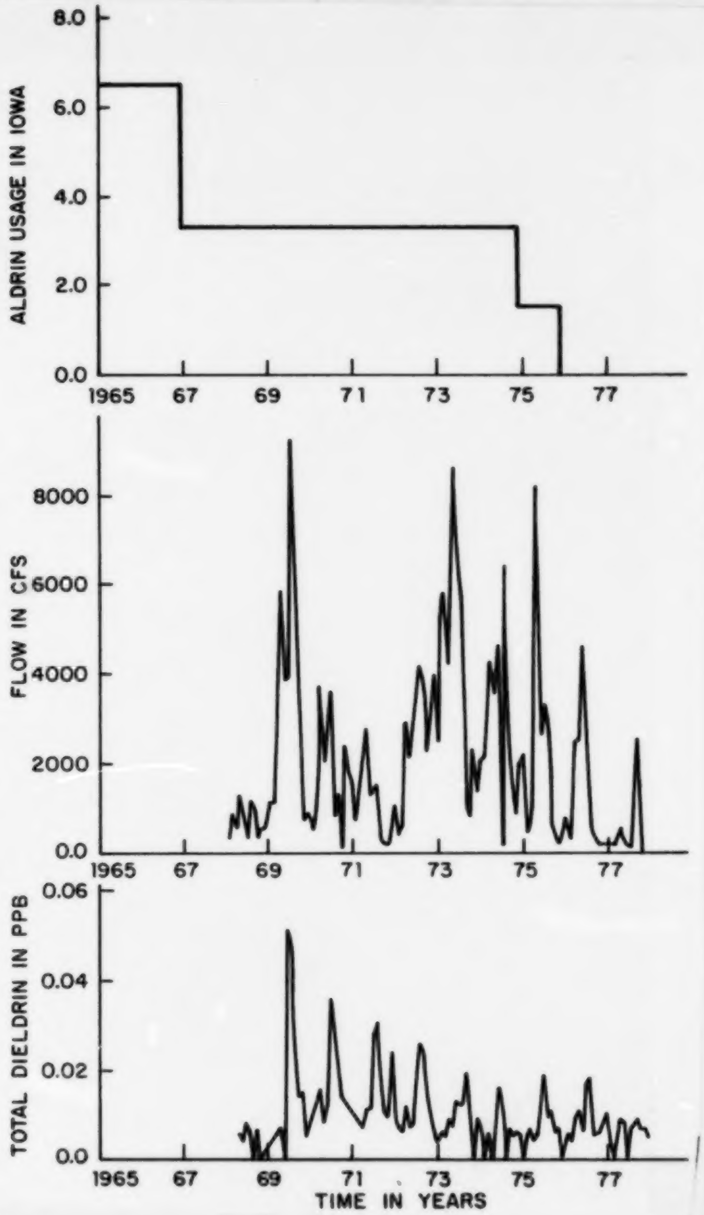

Figure II-1. Estimated Aldrin Usage (in million pounds) in Iowa and Total Dieldrin Concentrations in the Iowa River at Iowa City, 1968-1978

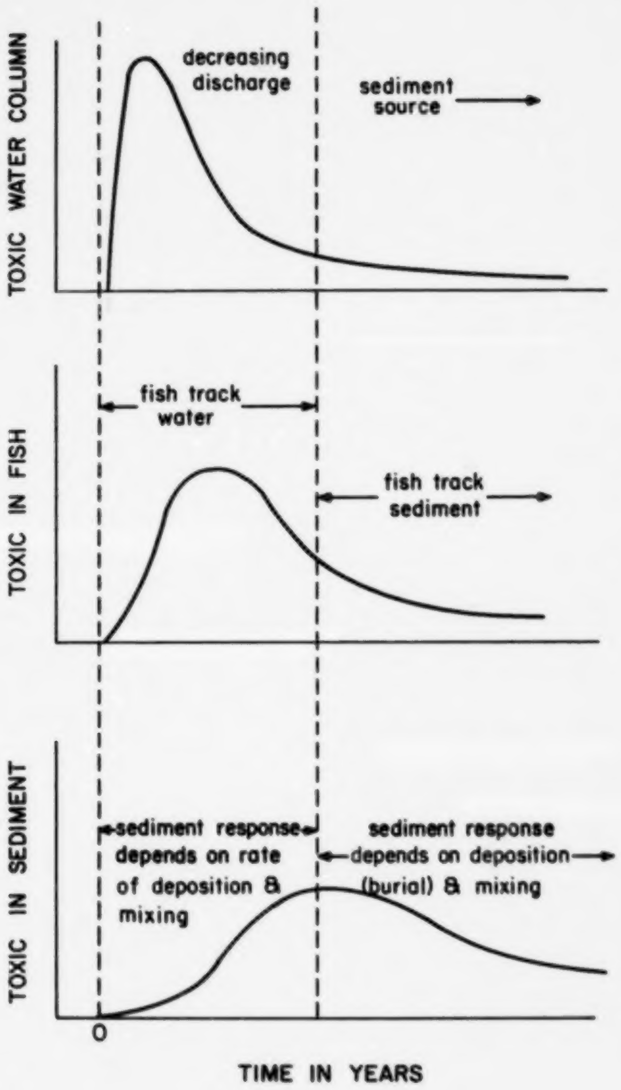

Figure II-2. Hypothetical Scenario for the Self-Purification of an Impoundment After the Introduction of a Hydrophobic Toxic Organic

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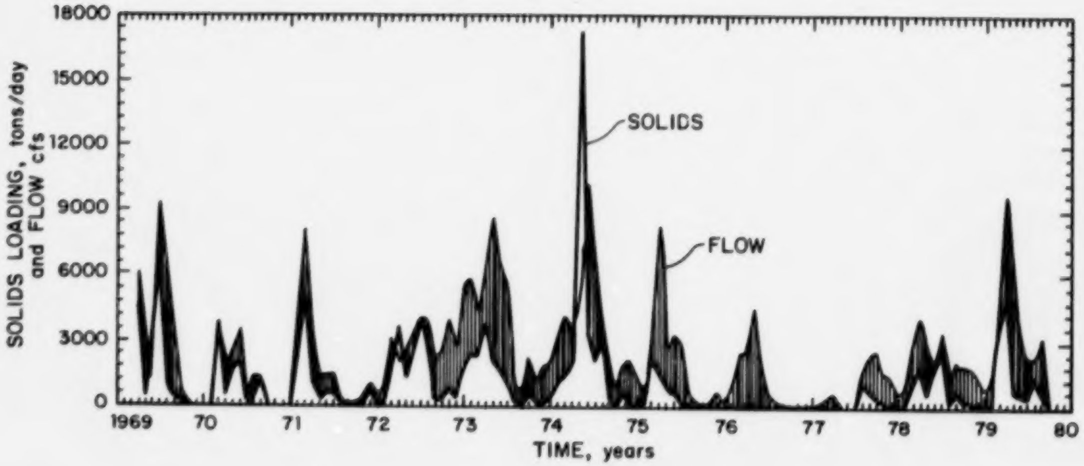

Figure II-3. Solids Loading and Flow Below Coralville Reservoir at Iowa City

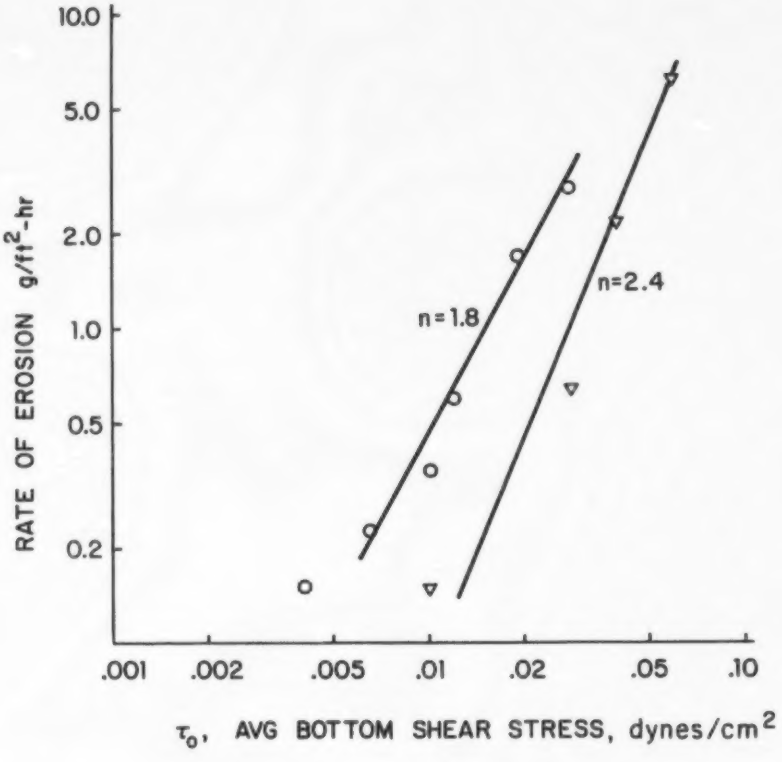

Figure II-4. Rate of Erosion versus Bottom Shear Stresses in dynes/cm^2 (calculated from data of Partheniades, 1965)

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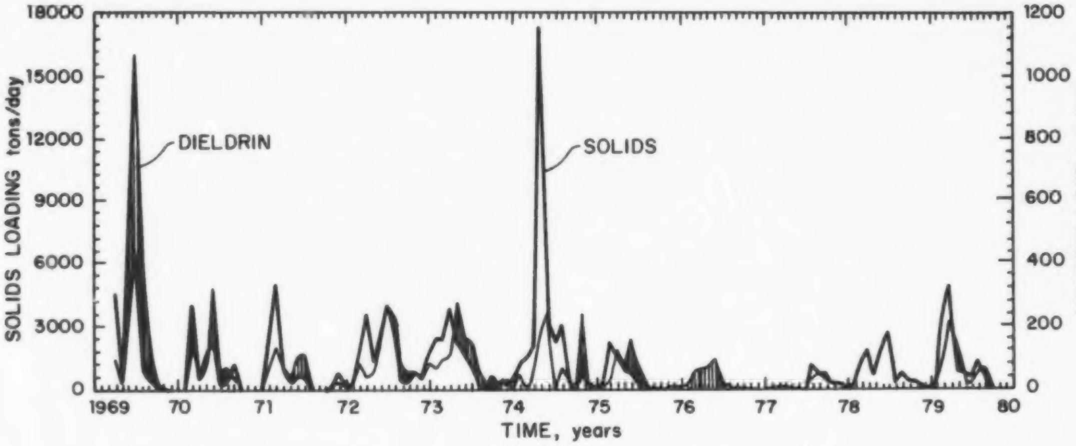

Figure II-5. Solids and Dieldrin Loading Below Coralville Reservoir at Iowa City (note: no dieldrin record exists for 1978)

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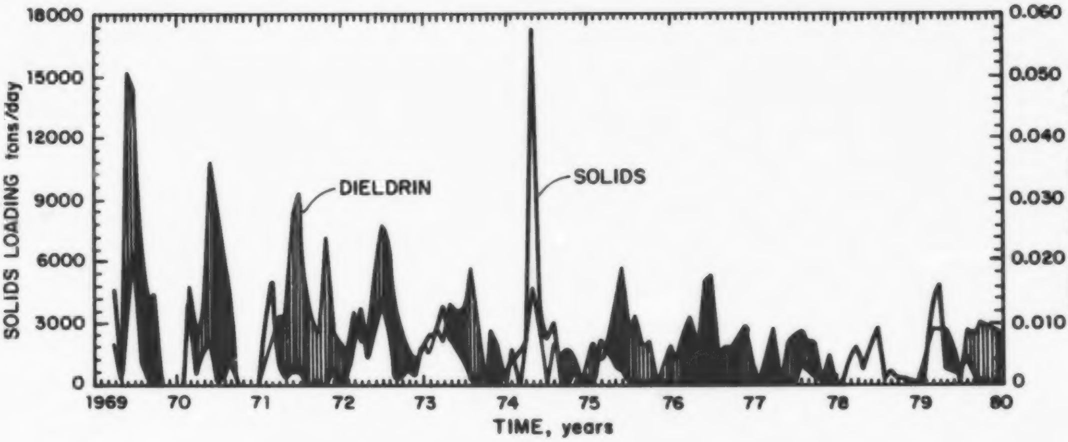

Figure II-6. Solids Loading and Total Dieldrin Concentration Below Coralville Reservoir at Iowa City (note: no dieldrin record exists for 1978)

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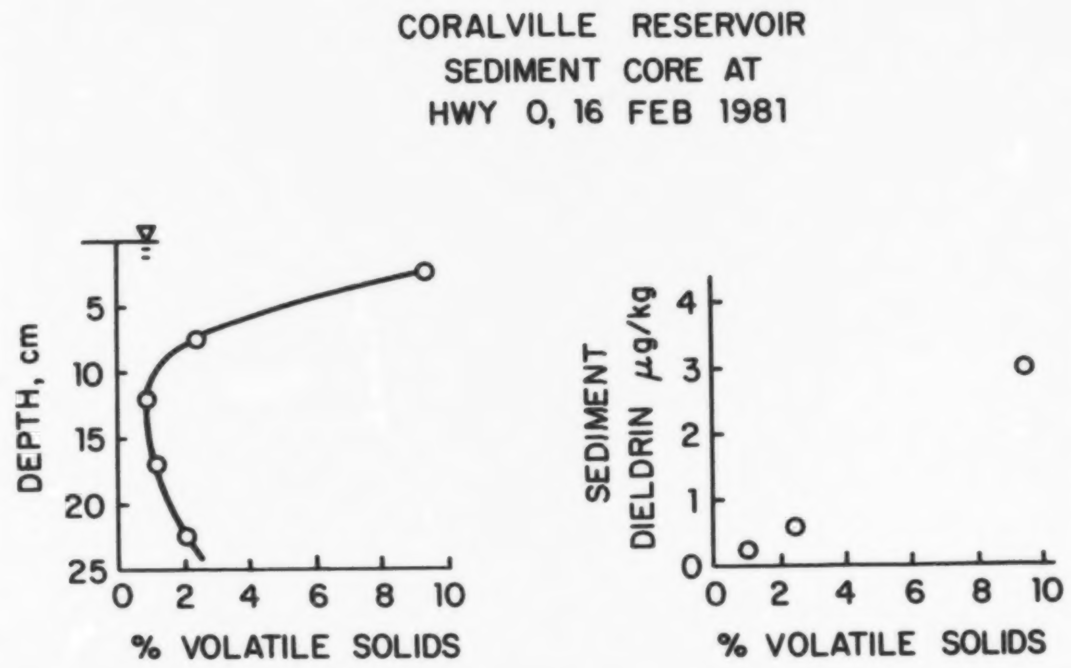

Figure II-7. Sediment Core Analyses for Percent Volatile Solids and Dieldrin Concentration Near the Inflow to Coralville Reservoir

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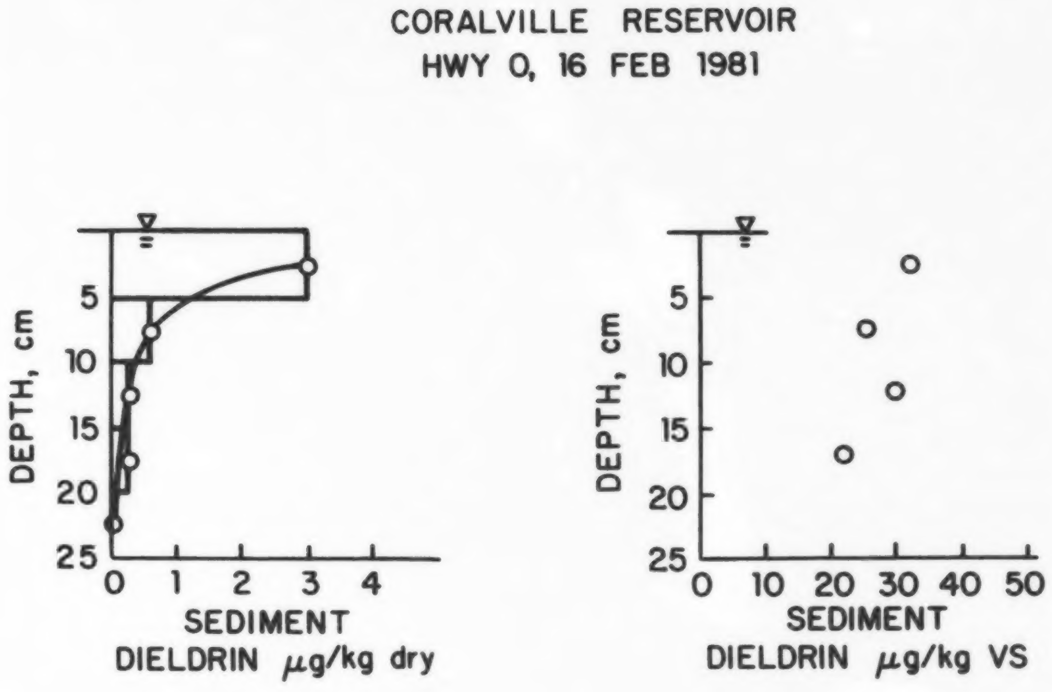

(a) (b)

Figure II-8. Sediment Core Analyses for Dieldrin Concentration on a Dry Weight Basis and on a Volatile Solids (VS) Basis

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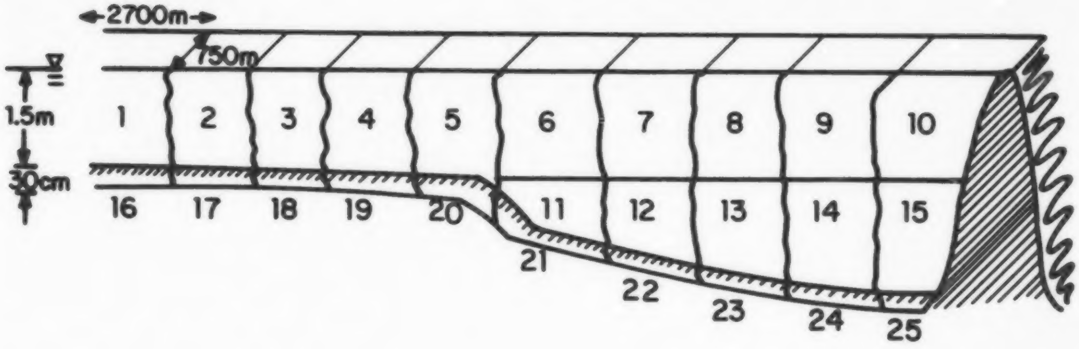
2700m
750m
1.5m
30cm
1
2
3
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Figure II-9. Compartmentalized Approach to Sediment - Water Interactions in Coralville Reservoir

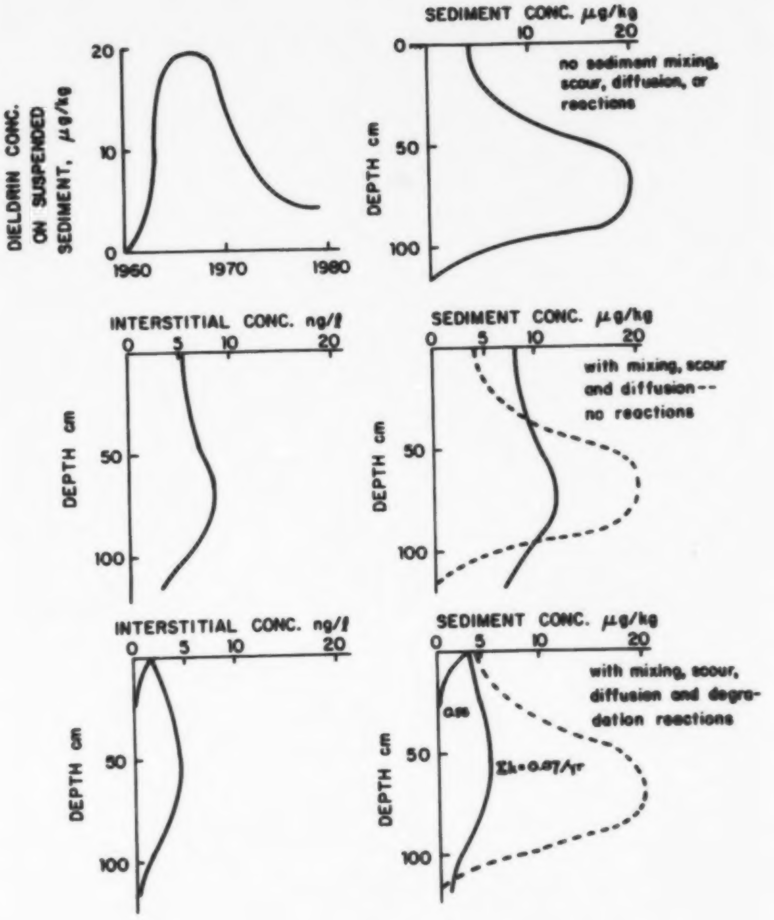

Figure II-10. Estimated Dieldrin Sediment Concentrations and Loading Scenario in Highly Depositional Zones of Coralville Reservoir

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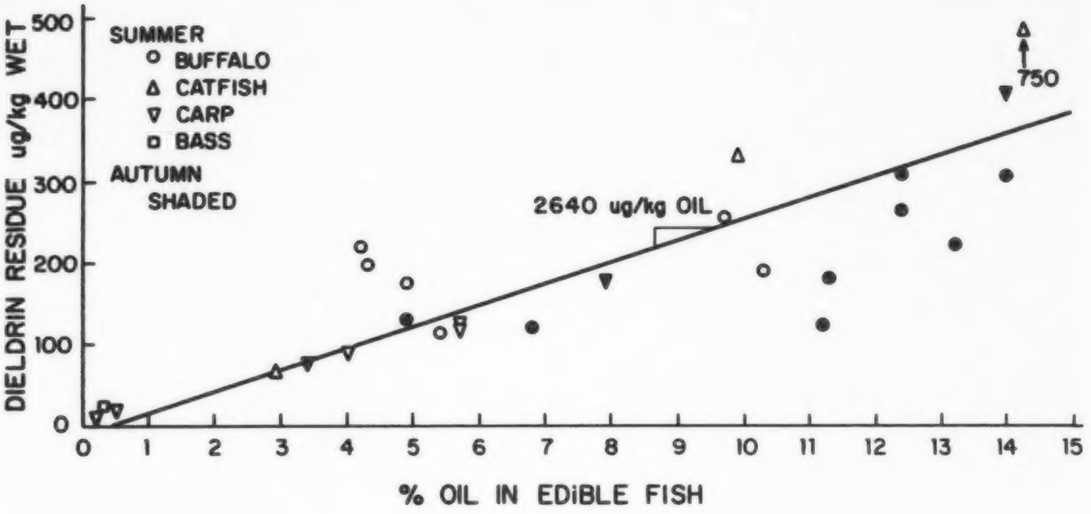

Figure II-11. Dieldrin Residues in Fish vs. Percent Oil Content, Coralville Reservoir, 1979 Field Data. Equation for Least squares regression: Y = 2640 X -10.8, r = 0.77.

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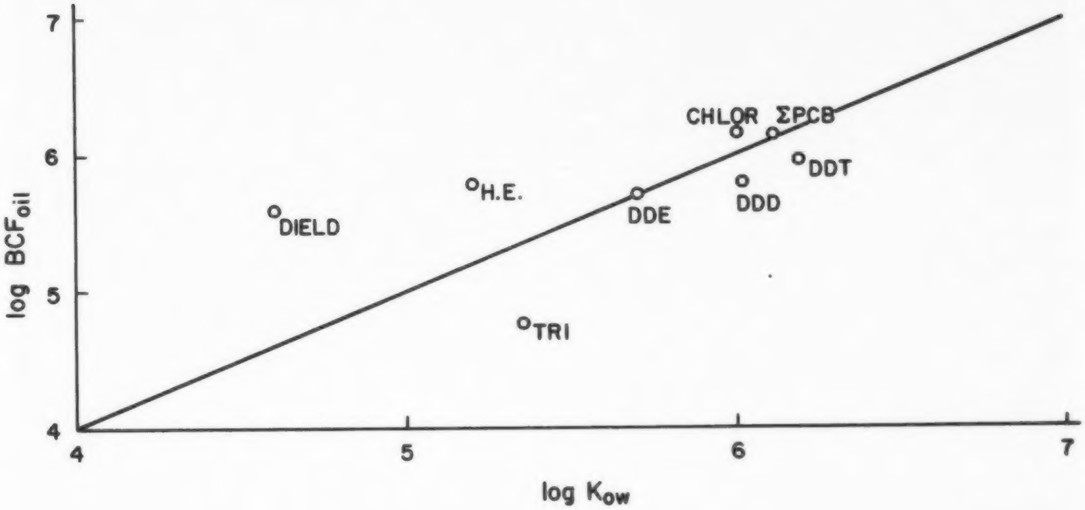

Figure II-12. Iowa Field Bioconcentration Factors in Fish Oil vs. Octanol/Water Partition Coefficients

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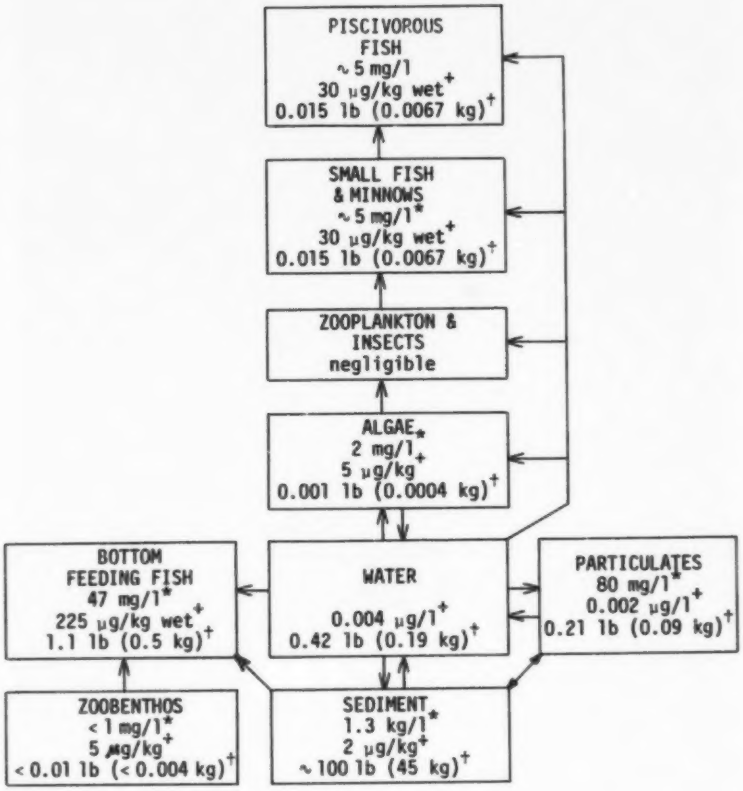
PISCIVOROUS FISH
~5 mg/l
30 μg/kg wet+
0.015 lb (0.0067 kg)†
SMALL FISH & MINNOWS
~5 mg/l*
30 μg/kg wet+
0.015 lb (0.0067 kg)†
ZOOPLANKTON & INSECTS
negligible
ALGAE*
2 mg/l
5 μg/kg+
0.001 lb (0.0004 kg)†
BOTTOM FEEDING FISH
47 mg/l*
225 μg/kg wet+
1.1 lb (0.5 kg)†
WATER
0.004 μg/l+
0.42 lb (0.19 kg)†
PARTICULATES
80 mg/l*
0.002 μg/l+
0.21 lb (0.09 kg)†
ZOOBENTHOS
< 1 mg/l*
5 μg/kg+
< 0.01 lb (< 0.004 kg)†
SEDIMENT*
1.3 kg/l*
2 μg/kg+
~100 lb (45 kg)†

---

*BIOMASS

+DIELDRIN CONCENTRATION

†DIELDRIN MASS

Figure II-13. Ecosystem Contamination Levels Based on Field Observations and Laboratory Microcosm Experiments

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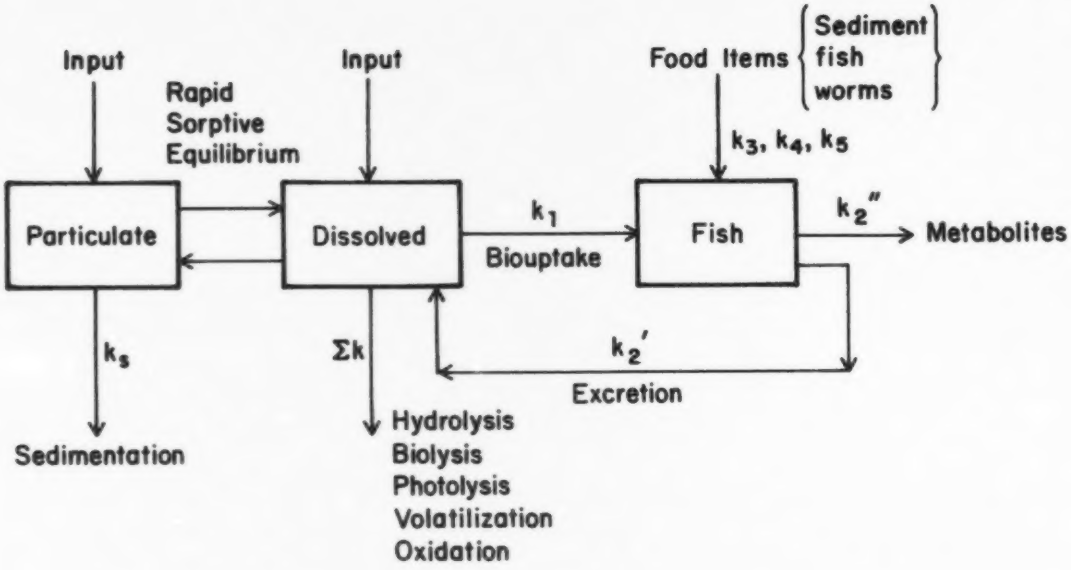
Input
Rapid Sorptive Equilibrium
Input
Food Items
Sediment
fish
worms
k_3, k_4, k_5
Particulate
Dissolved
k_1
Biouptake
Fish
k_2''
Metabolites
k_s
Sedimentation
Σk
Hydrolysis
Biolysis
Photolysis
Volatilization
Oxidation
k_2'
Excretion

Figure II-14. Bioaccumulation Model Schematic

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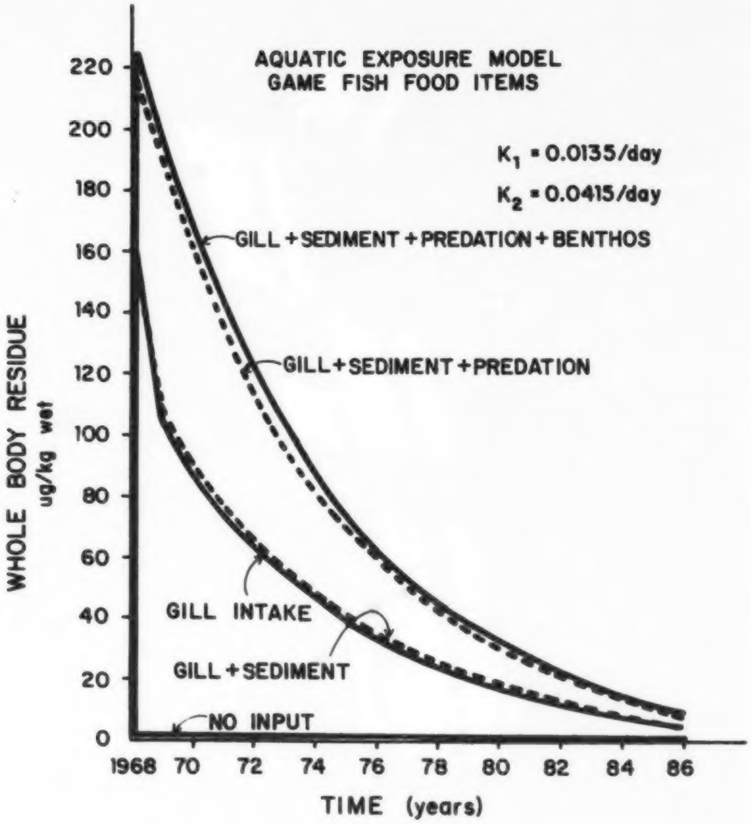

Figure II-15. Dieldrin Residues in Game Fish Simulation for Coralville Reservoir

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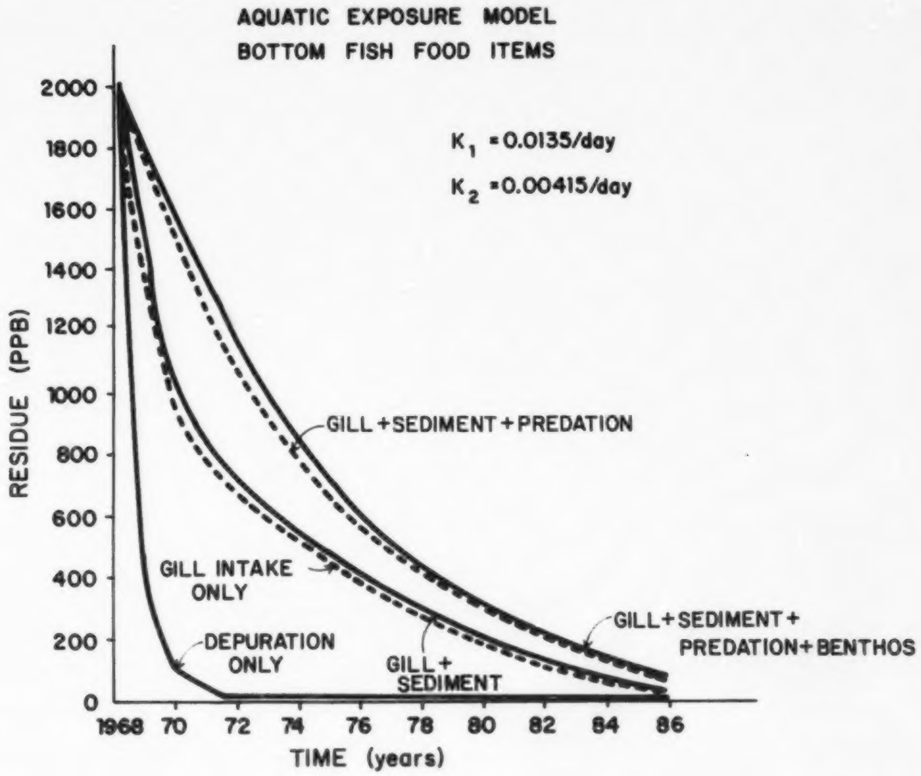

Figure II-16. Dieldrin Residues in Bottom - Feeding Fish for Coralville Reservoir

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CHAPTER III

A DYNAMIC SIMULATION MODEL FOR ALACHLOR AND ATRAZINE: FIELD VALIDATION USING MICROCOSM AND LABORATORY STUDIES

INTRODUCTION

One of the most widely used herbicides in the U.S. and Iowa is the soluble, acetanilide alachlor (Lasso®). It is applied at 1.1 kg/ha as a preemergent for grass control in corn during the period from mid-April to mid-May (see Tab. I-1 for structure). Concentration in Iowa waters range from 10-100 μg/ℓ in headwater streams with dilution and biodegradation accounting for lower concentrations (~1 μg/ℓ) in large rivers directly after application. It is a very water soluble herbicide (242 ppm) and has moderately low vapor pressure (2.2 x 10^{-5}mm Hg).

Other widely used herbicides in Iowa for broadleaf control are atrazine (Aatrex®) and cyanazine (Bladex®), both triazine herbicides. These herbicides are also quite soluble in water (33 and 150 ppm, respectively) and have low vapor pressures. Atrazine is applied at 0.5-0.8 kg/ha (active ingredient) from mid-April to mid-May. Concentrations in the Iowa River at Iowa City are 1-2 μg/ℓ during May-August. Concentrations of atrazine and cyanazine in the headwaters of the East Soldier River in Iowa were 54 and 130 μg/ℓ on 18 June, 1979.

The purpose of this study was to further test and validate the toxics model. A field validation was undertaken, and microcosm and laboratory studies were used to supplement the field data collection under spring runoff (time variable) conditions. One objective of the research was to determine if laboratory-derived rate constants could be used directly in a field validation effort. Soluble, biodegradeable chemicals were investigated to complement previous studies with dieldrin.

Field data on alachlor was gathered on Lake Rathbun, south-central Iowa reservoir on the Chariton River, by the University of Iowa Hygienic Laboratory [1]. The study was conducted during a high flow runoff period. Under these conditions, Lake Rathbun had a mean depth of approximately 29 feet, a mean hydraulic detention time of 162 days, and a mean volume of 351,000 acre-ft. Rathbun's 535 square mile watershed is primarily in row crop agriculture and pasture land.

MODEL DEVELOPMENT

The model uses a completely mixed flow-through system of one compartment. Equations 22 and 23 must be solved with a time variable mass loading

W(t) and detention time. The herbicides are approximately 99% in the dissolved phase such that the last term of Equation 23 is of little consequence. The time variable equation becomes a coupled set of ordinary differential equations shown below which were solved via a variable step size fourth order Runge-Kutta numerical technique.

$$\frac{dV}{dt} = Q_{in} - Q_{out} \tag{22}$$

$$\frac{d(VC_T)}{dt} = W(t) - Q_{out}\, C_T - \Sigma kCV - k_s C_p V \tag{23}$$

t = time, days

V = volume, ℓ

Q = flowrate, ℓ/day

C_T = total herbicide concentration, μg/ℓ

W = herbicide loading in mass per time, μg/day

k = sum of the pseudo-first order reaction rate constants in the dissolved phase, ℓ/day

k_s = sedimentation rate constant, ℓ/day

C_p = particulate herbicide concentration = K_pCM, μg/ℓ

C = dissolved herbicide concentration, μg/ℓ

Equation 23 must be differentiated by the chain rule:

$$\frac{d\,(VC_T)}{dt} = V\,\frac{dC_T}{dt} + C_T\,\frac{dV}{dt} \tag{24}$$

The final equation is:

$$\frac{dC_T}{dt} = \left\{Q_{in}\, C_{in} - Q_{out}\, C_T - \Sigma KCV(t) - K_s C_p\, V(t) - C_T\,\frac{dV}{dt}\right\} \cdot \frac{1}{V(t)} \tag{25}$$

Relationships between the total, particulate, and dissolved pesticide concentrations can be calculated assuming local equilibrium:

$$C = \frac{C_T}{1 + K_p M} \qquad (26)$$

$$C_p = \frac{K_p M C_T}{1 + K_p M} \qquad (27)$$

where M = suspended solids concentration, kg/ℓ

K_p = solids/water partition coefficient, μg/kg per μg/ℓ

GASP-IV Simulation Language

Ordinary differential equations can be easily coded into the simulation language GASP-IV. GASP-IV is a simulation language developed for handling discrete, continuous, and continuous/discrete time systems. The integration method provided by GASP-IV is a fourth order, variable step size Runge-Kutta routine for integrating systems of first-order, ordinary differential equations with initial values.

Equations 22 and 25 can be coded directly into GASP-IV as:

```
DD(1) = QIN - QOUT

DD(2) = (QIN*CIN - QOUT*SS(2) - SS(2)*DD(1))/SS(1)

                          - (KP*M/(1 + KP*M))*SS(2)*KS

                          - (1/(1 + KP*M))*SS(2)*K
```

where SS(1) ≡ V ; DD(1) ≡ dV/dt

SS(2) ≡ C_T ; DD(2) ≡ dC_T/dt

These equations are coded in subroutine STATE of GASP-IV. The initial conditions and the input values are set in subroutine INTLC. The values QIN, QOUT and CIN are obtained from a user-written FORTRAN function which looks up the values from a table with independent variable TNOW(=simulation time). Simulation for several pesticides can be performed simultaneously. (Their concentrations will be represented by SS(3), SS(4), etc.) Outputs are obtained in the form of a table and/or plot (with user-specified scale).

As an example of model validation, consider the herbicides atrazine and alachlor in an Iowa reservoir, Lake Rathbun. In order to assess the herbicide dynamics, a three step effort was undertaken including 1) biotransformation tests in natural waters, 2) microcosm testing, and 3) field data collection.

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MATERIALS AND METHODS

Biotransformation Tests

Biodegradation tests were performed in unfiltered Iowa River water with spiked additions of alachlor to 100-300 μg/ℓ under the following conditions: with and without bacterial seed from the Iowa River, with and without bacterial seed from treated soil, with and without nutrient additions, and during and after rainfall runoff events in the Iowa River. Controls were used to determine the extent of gas stripping, chemical hydrolysis, and sorption to glassware. Samples were aerated in the dark at ∿23°C.

A study of the microbial community was also performed during the degradation tests. Samples were spread-plated, incubated at 20°C for 7 days, counted at 10x magnification using a Quebec counter, and colony morphologies were recorded. Colonies were transferred to nutrient broth for 3 days at 20°C, observed and gram-strained and all morphologies were noted. In addition samples were streaked on BBL-brand MFC, M-Enterococcus, and M-Endo agars to test for fecal coliforms, fecal streptococci, and total coliform.

Microcosm Test

Fish used in this study were sunfish (*Lepomis sp.*) collected by shocking from the Coralville Reservoir on the Iowa River in early November, 1979. Algal growth was mostly *Microspora sp.* indigenous to the Iowa River. The alga became a test parameter by default after it choked out the macrophyte *potamogeton* orginally intended for use. Clams used were *Amblema sp.* collected by hand from a bed south of Fort Madison, Iowa, in Pool 19, Mississippi River during November, 1979. Sediment was collected from the same clam bed and used to cover the bottoms of the aquaria to a depth of about 4 inches. Water for the study was withdrawn from Iowa River influent to the University of Iowa Water Plant. Water quality varied greatly over the course of the two experimental phases. All equipment and organisms were arranged in a manner to simulate productive areas of the Mississippi River. Thirty fish and thirty clams were placed in each aquarium. Organisms were allowed to acclimate to the aquaria for a period of 2 weeks prior to beginning the herbicide experiment. Fish were fed a combination of live mealworms and commercial pellets as a supplement to natural food organisms present in the microcosm.

For the microcosm studies, Iowa River water was drawn into a 100 gallon cylindrical Nalgene tank and contaminants mixed in a batch process. Delivery to the aquaria was accomplished by means of a Masterflex peristaltic pump at 132 ml/min (∿ 50 gal/day). Aquaria were 55 gallon all-glass rectangular tanks (18" x 48" x 12") fitted with glass tubing at one end 1.5 inches from the top to allow positive overflow into a drainage system. Total water volume of the prepared aquaria was approximately 5 cubic feet or 37-40 gallons (140-150 liters) with a depth of 16 inches. Stable water temperature was maintained by two 200 watt aquarium heaters per tank. During the colder months, a temperature gradient resulting from the flow of cold influent into the warmer tank water was evident. Mixing was accomplished by placement of an airstone near the center of the tank. The photoperiod was automatically controlled with a 16 hour light and 8 hour dark cycle. Illumination was provided by two 40-watt fluorescent bulbs per aquaria which were suspended 5 cm (2-1/4") above the water surface. Alachlor was added as Lasso herbicide, the emulsifiable liquid, diluted in a carrier of acetone. Inflow concentrations averaged 8-10 μg/l but varied due to mixing conditions in the feed tank.

Field Tests

Samples were prepared, collected, and preserved according to Standard Methods for the Examination of Water and Wastewater, 14th edition and the Criteria for the National Pollutant Discharge Elimination System (NPDES). Grab samples were collected from four locations representing the two principal inflows from the Chariton River and South Chariton River, a depth-composite sample from Lake Rathbun, and a downstream sample. Weekly samples of water, fish, and sediment were analyzed for the herbicides alachlor, atrazine, and the insecticide dieldrin. The sampling period consisted of a series of runoff events from May-July, 1978. Flow was from guage records of the U.S. Geological Survey, and samples were analyzed by the University of Iowa Hygienic Laboratory.

RESULTS AND DISCUSSION

Biotransformation Test

Loss of alachlor by gas stripping proved to be a relatively small but detectable loss mechanism. The degradation rate was surprisingly independent of the source of inoculum, substrate or nutrient addition, and water quality. Zero order and first order kinetics fit the laboratory data well with rate constants of 6.4 μg/ℓ-day and 0.055/day, respectively. Second order kinetics did not hold very well since 100 fold increases in viable cells (as measured by the spread-plate technique in petri plates filled with BBL-brand nutrient agar) did not result in increased degradation rates. Paris et al. [2,3,4] have noted second order kinetics for biodegradation, first order in total cell count and first order in pesticide concentration.

Results are shown in Tab. III-1 from all of the biotransformation studies. The first order rate constants are in good agreement with those calcualted from Beestman and Deming [5] and those of Rao [6] for alachlor degradation in soil. An average half life of 12.6 days can be computed. The second order rate constant is quite variable, and is an order of magnitude larger than that determined in laboratory protocol measurements by Baughman and Paris at the USEPA Environmental Research Laboratory, Athens, Georgia (personal communication, 1980). However the procedures differ considerably and the USEPA measurement was a much shorter duration test (3-5 days).

A typical degradation curve (a semilog plot of concentration versus time) is shown in Fig. III-1. Usually a lag time of approximately 5-8 days was evident in which the degradation rate was low, followed by a more rapid and linear phase. Zero order kinetics also fit the experimental data quite well as reported by Pitter [7].

Results of the microbial community study indicated that spiked additions of alachlor, dextrose, or nutrients did promote significant changes in community structure, and that succession caused large changes in the taxa of controls during the course of the degradation experiments. This technique also demonstrated a source of bacterial contamination coming through the filtered air supply [8].

Microcosm Test

Results from the microcosm experiment are shown in Fig. III-2 and 3 [9]. Alachlor and atrazine were not detected in fish, sediments, clams, or algae probably due to their low octanol/water partitioning and rapid metabolic transformations. After 30 days, the feed solution was changed to settled river water, and washout of herbicides was observed from day 30-60. The percent of alachlor removed during the experiment was approximately 35% (Fig. III-2). At near steady state (days 15-30) the removal was also ∿35%. Therefore it is possible to estimate the degradation rate for a system with a 0.8 day dentention time to be 0.67/day. This is much greater than the estimated 0.055/day from the biotransformation study. This points up the need for similarity in laboratory microcosms. Microcosms should have the same ratios of biomass-to-volume and production-to-biomass ratios in order to mimic the ecosystem. In this case, the large mass of algae which developed and the large biomass was probably responsible for the rapid loss of herbicides due to sorption and biotransformations. Algae are known to biodegrade many organics and herbicides. Atrazine was ∿40% removed in the microcosm study, also indicating sorption and possible biotransformation (Fig. III-3).

Field Tests

Modeling efforts on Rathbun Reservoir in Iowa for the herbicides alachlor and atrazine are much different than for hydrophobic pollutants. Being quite soluble, these herbicides are shown to undergo negligible sedimentation but to biologically degrade and to be transported out of the Reservoirs via the outflow. Figs. III-4-7 are the results for alachlor in Rathbun Reservoir. Time-variable loadings and flow were required to accurately model in-situ and outflow concentration data. The rate of degradation in Fig. III-7 was significant, and the pseudo-first order biodegradaton rate constant was 0.04 per day, in relative agreement with laboratory biotransformation measurements. Equations 22 and 25 were solved simultaneously to plot the results shown in Fig. III-7. At least for the case of alachlor in Rathbun Reservoir, the use of a laboratory-derived biotransformation rate would have been appropriate for modeling purposes.

The results for atrazine in Lake Rathbun are less satisfying. Literature values for atrazine degradation in soils and waters range from 0.01-0.05/day. Using the lowest of these literature values (0.01/day) and the measured input concentrations of Fig. III-8, the calculated concentration is less than the 0.5-1.2 μg/ℓ measured Lake concentration (Fig. III-9). The model results of Fig. III-9 use double the measured inputs in order to fit the field data. The reason that model results do not reflect the field data cannot immediately be attributed to channeling or incomplete mixing because the alachlor mass balance worked nicely (Fig. III-7). Possible other reasons include: 1) an unmeasured source of atrazine such as overland runoff or bed sediment, and 2) analytical chemistry problems at these very low concentrations, near the detection limit of 0.2 μg/ℓ.

For comparison a final simulation was performed for dieldrin in Lake Rathbun. Measured inflow concentrations used as model input (Fig. III-10) and results are plotted in Fig. III-11. Once again model results are lower than measured values. However these concentrations range from 0.4-1.0 ng/ℓ and are extremely low.

An observation is that one should not search for the biological effects of pesticides in large rivers and reservoirs. It is the headwaters and small tributaries which have 50-100 fold higher exposure concentrations. It is also the tributaries which often have the most habitat diversity and hence species diversity and which provide spawning areas for fish. Nevertheless, the pesticide concentrations found in Iowa during the tenure of this research are well below all acute toxic thresholds and LD_{50} values.

This field validation demonstrates the use of laboratory measurements in a modeling framework. A further improvement would be to track the daughter products of herbicide biodegradation as well as the parent compound. It is worth noting that approximately 75-90% of the transport occurs over less than 20% of the time. Due to the transient nature of runoff events, it is necessary to perform time variable simulations in order to accurately represent the mass fluxes as well as concentrations. Annual average or steady state representations are not accurate in these cases.

SUMMARY

Laboratory biotransformation and microcosm studies were helpful in predicting the dynamics of alachlor and atrazine in Lake Rathbun. Model predictions were within a factor of five for atrazine, a factor of two for dieldrin, and a factor of one for alachlor. For most purposes, these would be acceptable simulations and the model should be considered as field-validated. In these simulations, there was no adjustment of the rate constants made to fit the field data -- there was no calibration or model tuning. Laboratory and literature rate constants were used directly in a comparison with field observations.

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Table III-1

KINETIC BIODEGRADATION RATE CONSTANTS

Sample	Alachlor Initial Conc. (µg/1)	Zero Order k" (µg/1-day)	Zero Order r	1st Order k' (day^{-1})	1st Order r	2nd Order Rate (X10^{-10}) (1/org.-day)[a]	Microbe Conc. (X10^{6}) (orgs./1)[b]
After Rain, no nutrients	226.4	8.10	-0.99	0.071	-0.99	5.3	135 ± 104
After Rain, dextrose	226.4	7.83	-0.98	0.062	-0.97	15.4	40 ± 39
After Rain, dextrose, N&P	226.4	7.91	-0.99	0.048	-0.99	2.5	195 ± 121
Before Rain, dextrose	218.7	6.20	-0.97	0.023	-0.96	3.5	69 ± 70
Before Rain, dextrose, N&P	218.7	6.12	-0.99	0.044	-0.99	6.7	66 ± 39
River Water	244.5	6.88	-0.99	0.030	-0.97	6.4	45 ± 40
Reservoir Water	213.5	3.68	-0.98	0.021	-0.97	20.7	10 ± 11
Sediment/Res. Water	247.1	8.01	-0.98	0.074	-0.99	8.1	91 ± 49
Activated Sludge/R.W.	277.8	7.20	-0.97	0.046	-0.98	5.7	79 ± 41
Soil 2/River Water	264.4	7.94	-0.99	0.060	-0.98	11.3	53 ± 32
Soil 1/River Water	144.6	4.20	-0.99	0.062	-0.98	0.1	5000 ± 1908
1/8 Inoculum/Riv. Water	128.7	5.26	-0.99	0.083	-0.99	11.3	73 ± 68
3/4 Inoculum/Riv. Water	114.2	3.98	-0.97	0.099	-0.99	3.5	280 ± 176
Mean		6.41 ± 1.65		0.055 ± 0.023		7.7 ± 4.4	
Coefficient of Variation (X100)		25.7		41.8		56.4	
Geometric Mean		6.11		0.051		5.07	

[a] $k = \frac{k'}{X}$

[b] Concentration is averaged for linear portion of degradation over the time period for which 1st order calculations were made

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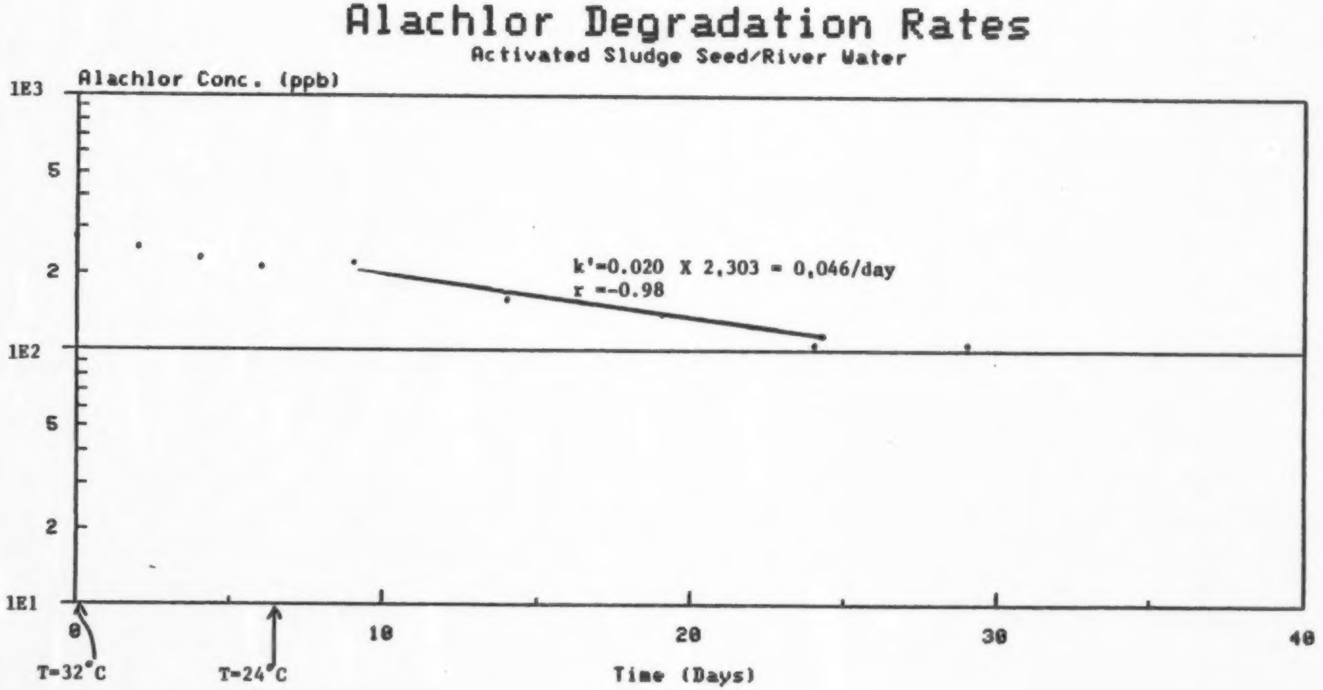

Figure III-1. Alachlor Degradation in Iowa River Water with an Activated Sludge Innoculum

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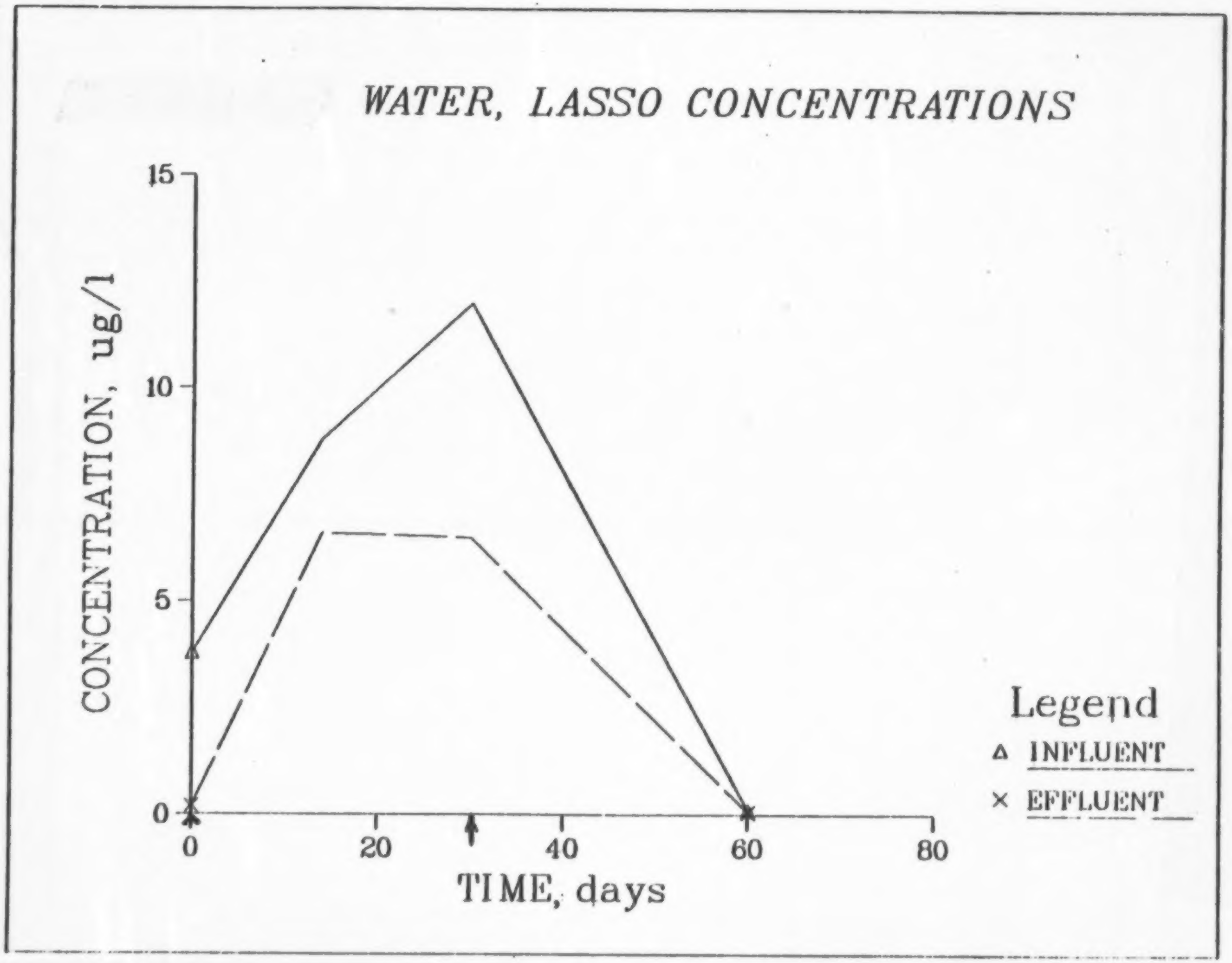

Figure III-2. Alachlor Microcosm Concentrations in External Water Samples

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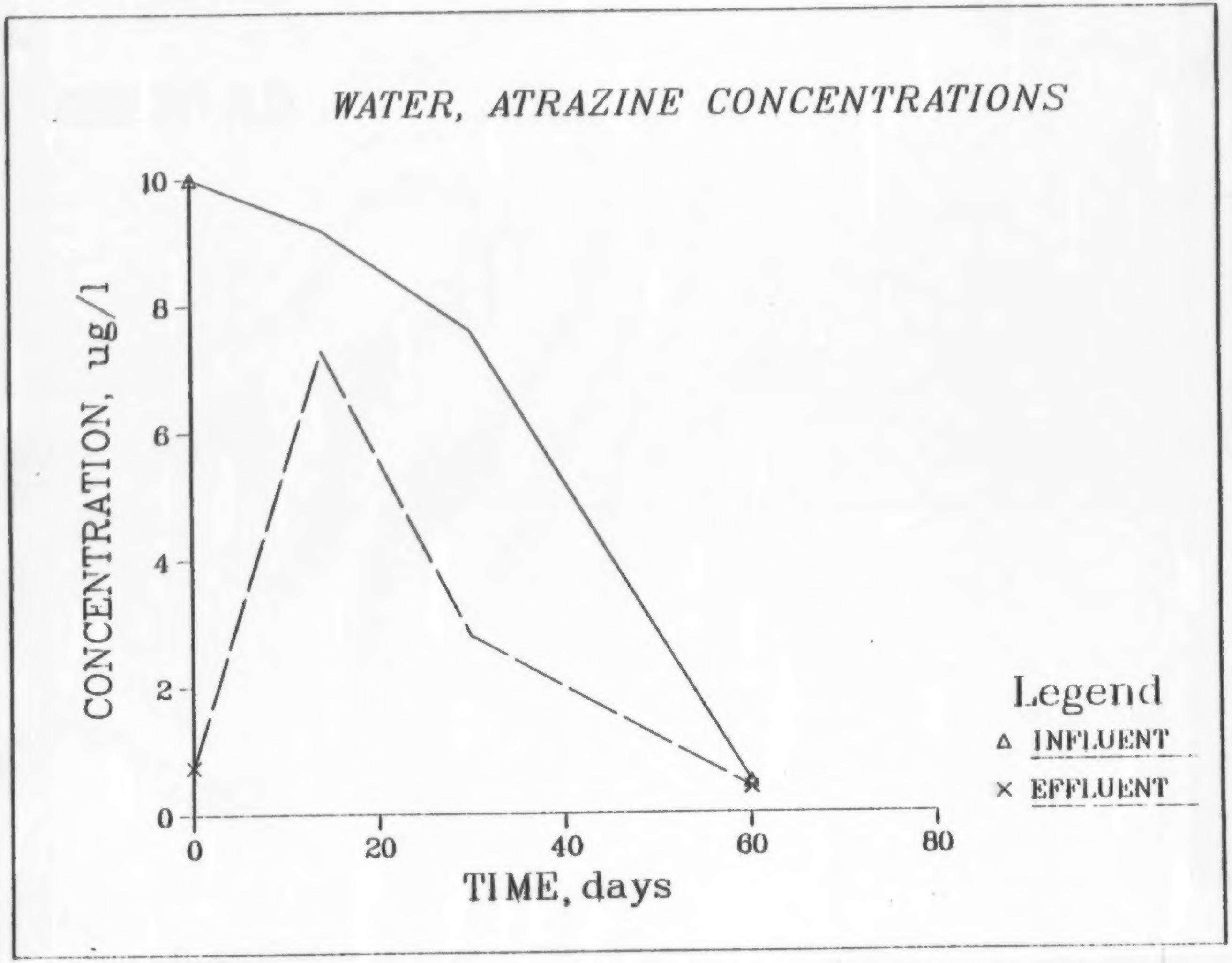

Figure [illegible] Atrazine Concentrations in Filtered Water Samples

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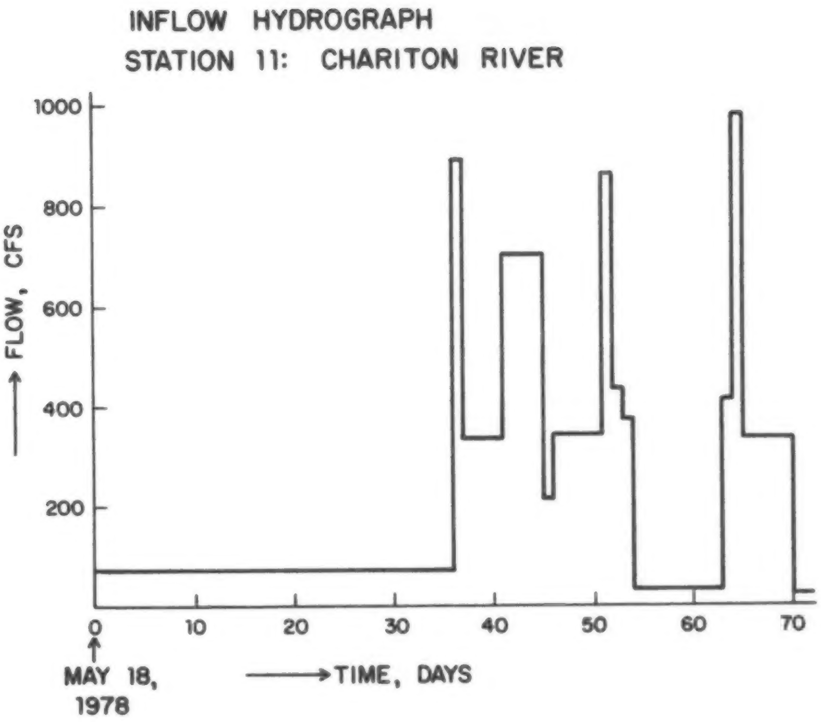

Figure III-4. Model Inflow to Lake Rathbun

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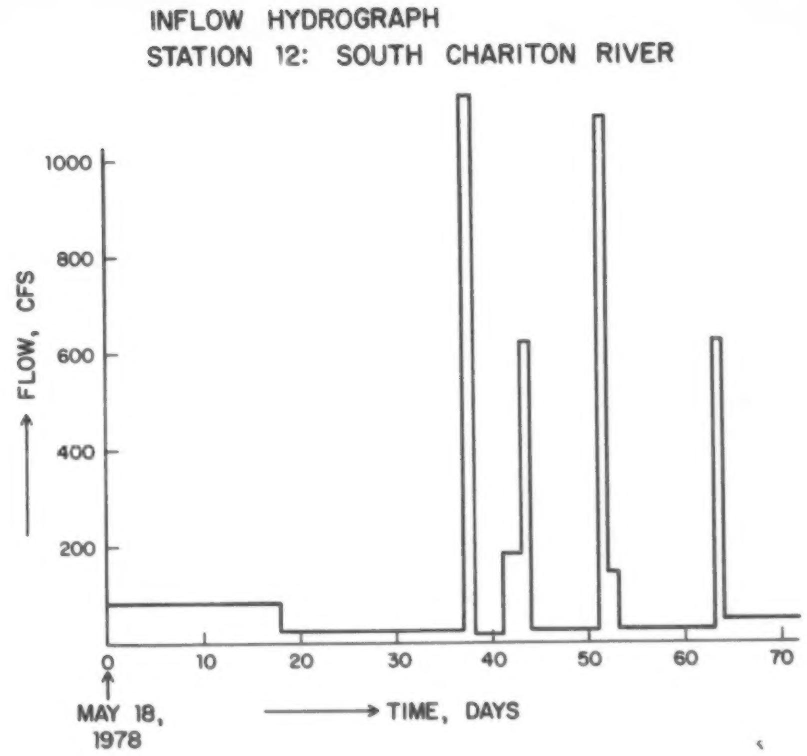

Figure III-5. Model Inflow to Lake Rathbun

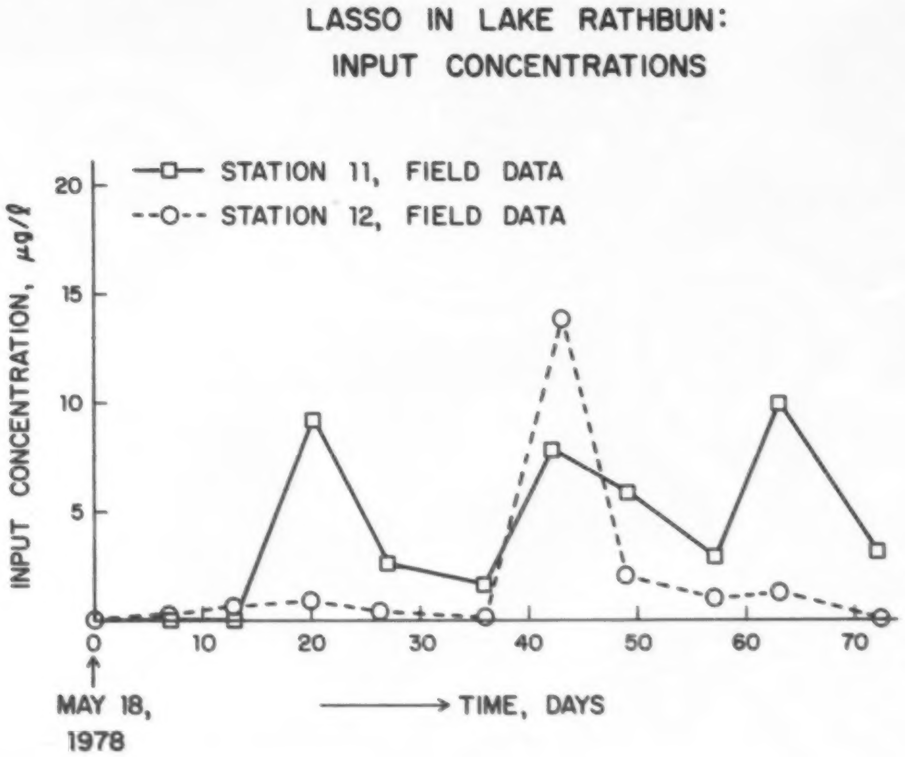

Figure III-6. Measured Alachlor Inflow Concentrations and Model Input

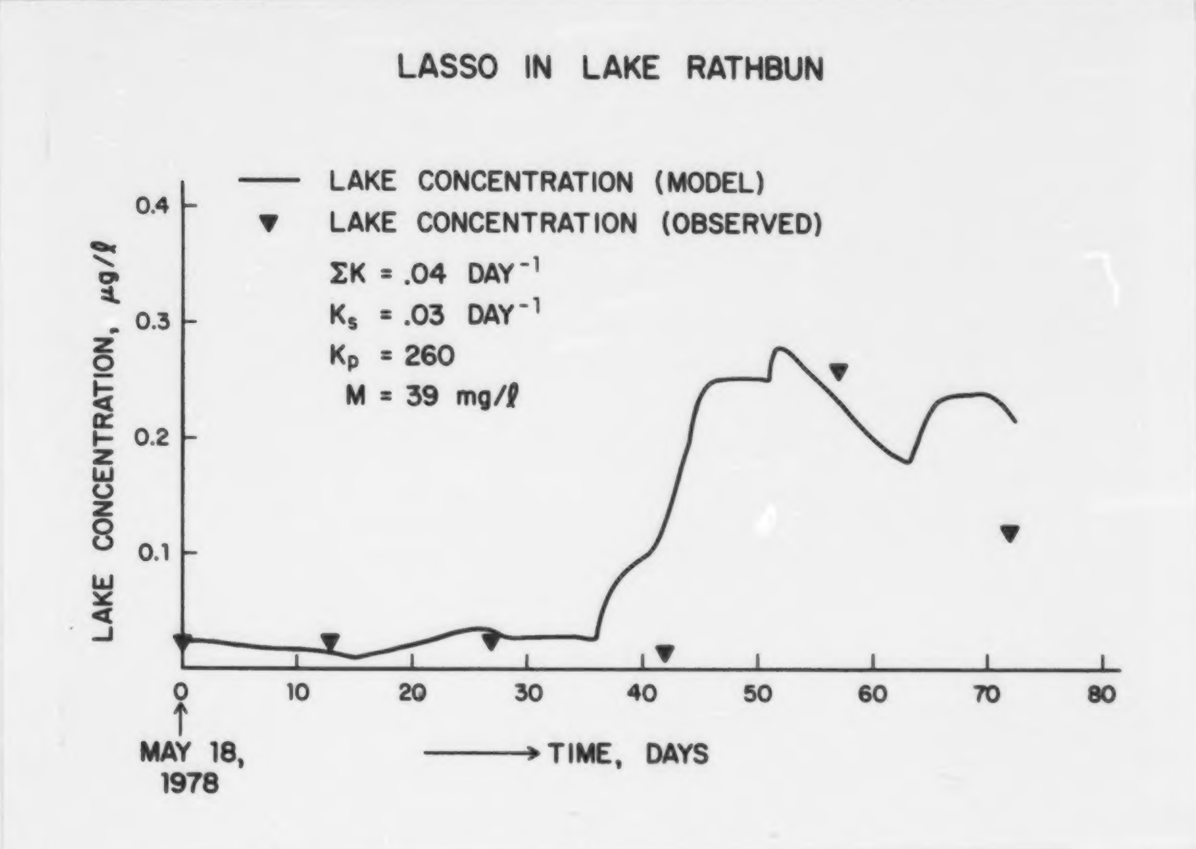

Figure III-7. Model Results and Measured Alachlor Concentrations in Lake Rathbun, 1978

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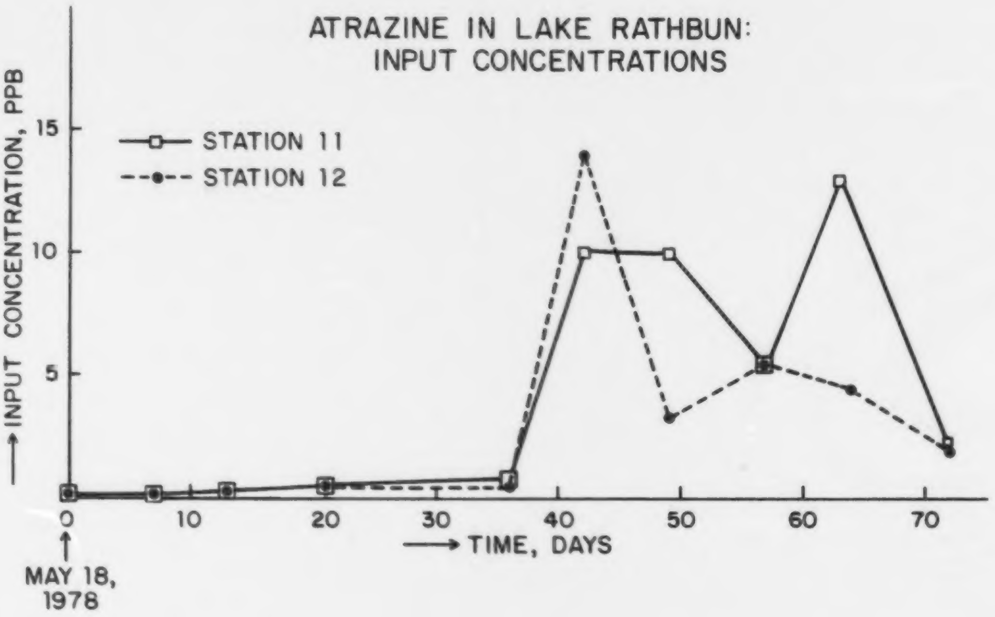

Figure III-8. Measured Atrazine Concentrations and Model Input

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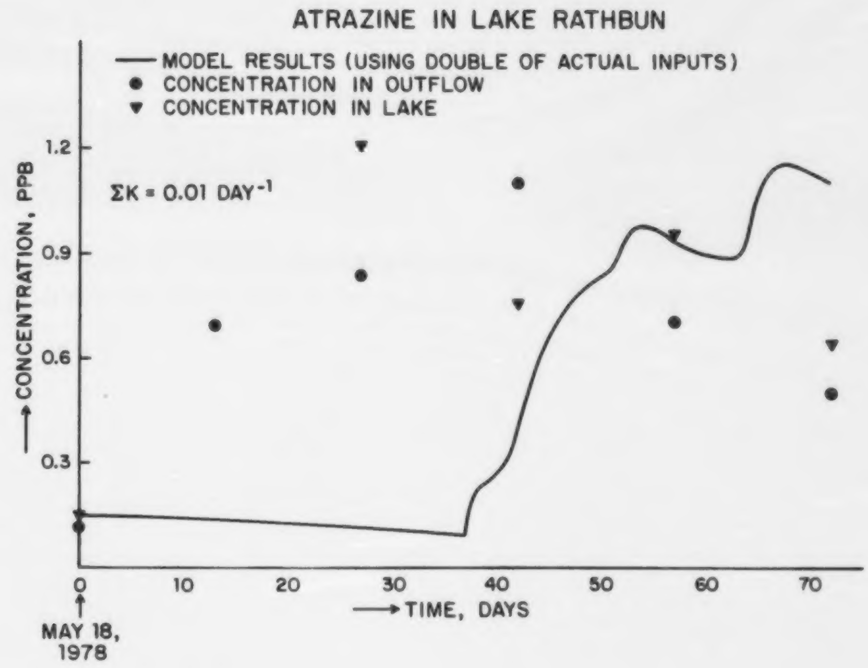

Figure III-9. Model Results and Measured Atrazine Concentrations

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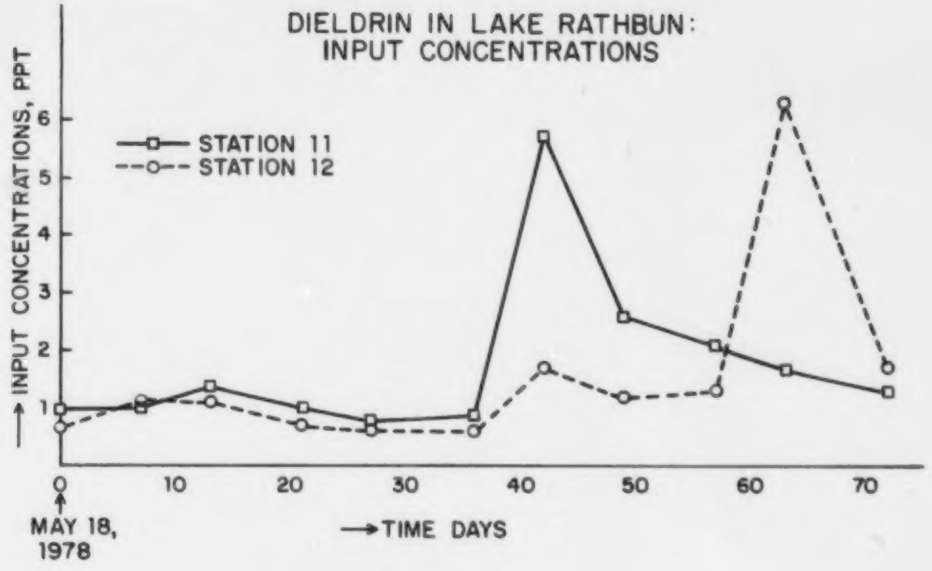

Figure III-10. Measured Dieldrin Concentrations and Model Input

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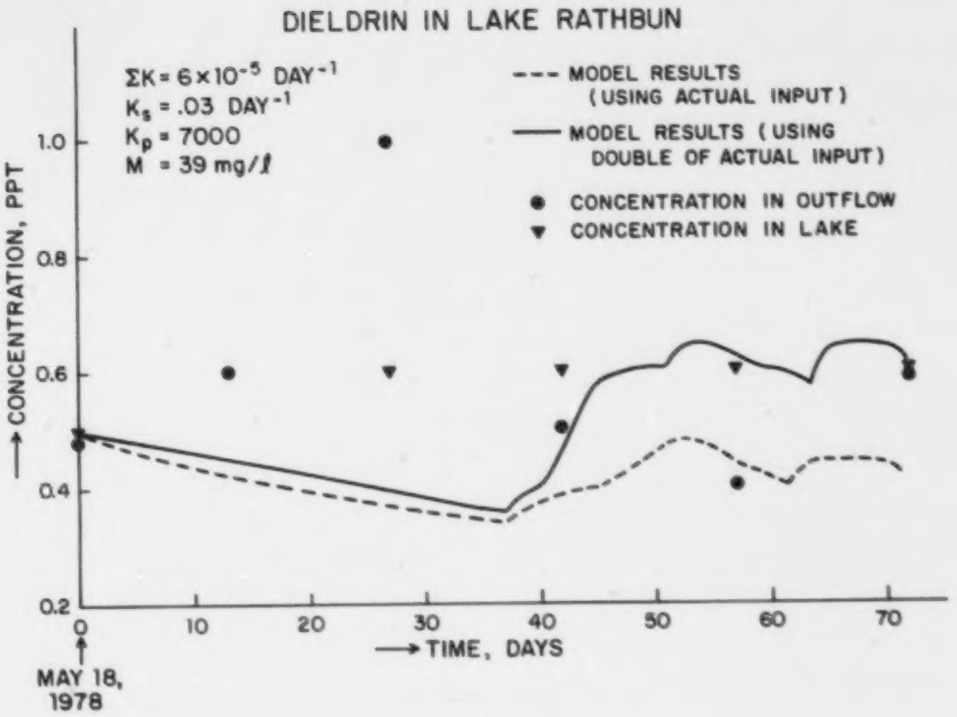

Figure III-11. Model Results and Measured Dieldrin Concentrations

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CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS

CONCLUSIONS

The model TOXIC (and versions thereof) has been calibrated with Iowa reservoir data for the insecticide dieldrin and the herbicides alachlor and atrazine. Steady state analyses and quasi-dynamic simulations with time-variable flows and loadings have been accomplished. Model coefficients were derived from laboratory data and in some cases literature data.

For the herbicide alachlor, laboratory protocol measurements were used directly in model simulations with excellent agreement between model predictions and measured concentrations. Thus the model may be considered field-validated. Laboratory measurements were used in simulations of alachlor, atrazine and dieldrin, and results were generally within an order-of-magnitude of field data.

Of course the toxic substance model described in this report can still be improved. It can certainly be made more mechanistic and complicated, but the law of diminishing returns will apply in further endeavors. It is somewhat difficult to speak of a validated model code -- we gain confidence in the model structure and code with each new and successful application. A new calibration and verification is necessary for each new chemical which tests each new feature of the model TOXIC. In this research the model has been successfully tested for three toxic chemicals under a variety of conditions and locations.

One of the most important aspects of the dieldrin simulations in Chapters II and III was the choice of time scale and space scale. Especially in quasi-dynamic applications, where one variable varies in time and space while another is held constant, averaging problems arise. To simulate both the exposure concentration and mass fluxes accurately, one must use a fully dynamic, spatially variable model in which flow, suspended solids, toxicant concentration, pH, and other state variables are functions of time and space. Fortunately most applications do not require such accuracy, and we may settle for steady state or quasi-dynamic models such as TOXIC. TOXIC was utilized in a management decision by the Iowa Conservation Commission to lift the ban on commerical fishing in Coralville Reservoir in 1979.

Sediment has been a small net source of dieldrin to the water column of Coralville Reservoir, especially important under low flow conditions. Coralville Reservoir contains approximately 100 lbs of dieldrin in the sediment. It will take 6-10 more years to achieve less than detectable

(<0.002 μg/ℓ) dieldrin in the water column, primarily due to continued inflow as well as sediment desorption.

Lastly, field bioconcentration factors when normalized on a lipid basis were approximately equal to laboratory-derived bioconcentration factors similarly weighted. The bioconcentration factors were also proportional to the octanol water partition coefficient. Bioconcentration is the primary mode of pesticide uptake in Coralville Reservoir and food items are generally of less importance.

RECOMMENDATIONS

The following recommendations are offered

1) Reactions in the sediment phase, especially biotransformations and sediment catalyzed reactions, are critical to model results. This is an area of future research needs.

2) Most hydrophobic toxics are intimately connected with the solids balance. More research is needed in the area of sediment transport, especially of cohesive sediments.

3) Chronic biological effects should be examined in headwater streams where nonpoint source runoff concentrations are large and diversity is high. Modeling will require a fully dynamic approach.

The key to modeling toxic chemicals is not unlike that for the conventional pollutants: one needs a tight water budget, a knowledge of mixing characteristics, a good solids balance, and accurate reaction kinetics.

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APPENDIX

TOXIC Documentation
Program Codes
Sample Input
Sample Outputs

TOXIC, A multicompartment pesticide simulation model

TOXIC is a 30 compartment pesticide simulation model. It is mainly intended for simulating one pesticide in a reservoir. TOXIC considers the aquatic system being simulated as being divided into a number of compartments, not exceeding 30. Each compartment is considered to be a completely mixed system. The concentration of pesticide through time is described by a set of ordinary differential equations, one for each compartment. The equations are integrated by the Runge-Kutta fourth order method to result in a simulation.

The inputs to the model can be classified under the following categories:

1. Geometric properties, such as volumes of compartments, distances between them, surface areas, and locations with respect to other compartments
2. Flows between compartments, and between each compartment and the outside of the system
3. Reaction rates, settling rate constants, and partition coefficients
4. Solids concentrations in each compartment
5. Bulk dispersion coefficients between compartments
6. Simulation parameters such as step size and time of simulation.

The solids concentration in each compartment is obtained from another model called SOLIDS. SOLIDS is similar to TOXIC in every way except that only solids are simulated. The input for the solids model are 1,2,5 and 6 above.

The subroutines involved in TOXIC are:

1. The main program.
   The main program reads in all the input data. All reaction rates and flows are initialized to zero. The input is in free format, therefore only the non zero elements need to specified. The main program also checks for a flow balance on each compartment within an error of 5%. If the flows do not balance, it calls subroutine ERROR which prints out an error message. If errors are found in the input data, simulation is not attempted. If no errors are found, the main program calls subroutine SOLVE which performs the integration. The main program also echo checks the reaction rates and prints the fractions in the dissolved and suspended phases for each compartment. Other input data is echo checked on request.

2. Subroutine ERROR.
   This subroutine prints out error messages and keeps a count on flow balance errors.

3. Subroutine PRINT.
   This subroutine echo checks the input data on request.

4. Subroutine SOLVE.
   This is the executive routine which performs the integration.

5. Subroutine DIFFEQ.
   This subroutine sets up the differential equations for each compartment. It is called by SOLVE several times during each integration step.

6. Subroutine INPUTS.
   This subroutine is called by subroutine SOLVE at the beginning of each integration step. INPUTS has to be provided by the user, and contains any exogenous inputs to the sytem such as concentrations in inflows.

COMMON BLOCKS

The common blocks used in TOXIC are:

```
 COMMON /GEN/ NUM,H,OUTDEL,TFIN,TIM,NERR,NOUT,INTER

 COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30),IPOS(30,30),
1ED(30,30),EP(30,30),SA(30,30),AL(30,30),DISP(30,30),DISD(30,30)

 COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30),PC(30)

 COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)

 COMMON /REAC1/ AQY(30),AKI(30),AKP(30),OXK(30),RO2(30),AKO(30),
1BKB(30),AKA(30),AKN(30),PH(30),AKH(30),AKV(30),GRM(30),YLK(30),
2HKS(30),XMB(30),AKB(30)

 COMMON /REAC2/ OXKP(30),RO2P(30),AKOP(30),BKBP(30),AKNP(30),
1PHP(30),AKPH(30),GRMP(30),YLKP(30),HKSP(30),XMBP(30),AKBP(30)
```

Each of the variables in these common blocks will be explained now.

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COMMON /GEN/ NUM,H,OUTDEL,TFIN,TIMNERR,NOUT,INTER

Variable	Description	Provided by:
NUM	Number of compartments in system.	User
H	Step size for integration, days.	User
OUTDEL	Time between storage of output, days.	User
TFIN	Time of simulation, days.	User
TIM	Current simulation time, days.	Computed
NERR	Number of errors in input days.	Computed
NOUT	Number of output points.	Computed
INTER	Indicator for printing fluxes between compartments. = 1 : print fluxes = 2 : do not print fluxes	User

This common block is used to specify general simulation parameters.

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      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30),IPOS(30,30),
     1ED(30,30),EP(30,30),SA(30,30),AL(30,30),DISD(30,30),DISP(30,30)
```

Variable	Description		Provided by:
V(I)	Volume of compartment I,	Mm^3*	User
QIN(I)	Inflow to compartment I from outside the system,	Mm^3/day	User
QOUT(I)	Outflow from compartment I to outside the system,	Mm^3/day	User
Q(I,J)	Flow from compartment I to compartment J,	Mm^3/day	User
IPOS(I,J)	=1: compartment I is above comp. J =0: compartment I not above comp. J		User
ED(I,J)	Dispersion coefficient for dissolved phase between compartment I and compartment J,	m^2/day	User
EP(I,J)	Dispersion coefficient for particulate phase between compartment I and compartment J,	m^2/day	User
SA(I,J)	Surface area between compartment I and compartment J,	km^2	User
AL(I,J)	Mean distance between compartment I and compartment J,	m	User
DISD(I,J)	ED(I,J)*SA(I,J)/AL(I,J)		Computed
DISP(I,J)	EP(I,J)*SA(I,J)/AL(I,J)		Computed

$^*Mm^3 \equiv 10^6\ m^3$

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(4-76)

```
COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30),PC(30)
```

Variable	Description		Provided by:
AM(I)	Mass of solids in compartment I	kg/l	User
AMIN(I)*	Mass of solids in inflow for compartment I	kg/l	User
DAM(I)*	Derivative of AM(I)	kg/l-day	Computed
AKS(I)	Settling rate constant for compartment I	1/day	User
PC(I)	Partition coefficient for compartment I	ℓ/kg	User

*Used only for the solids balance model.

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BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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```
COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
```

Variable	Description		Provided by:
C(I)	Concentration of pesticide in compartment I,	μg/l	Computed (Initial values are user provided)
CIN(I)	Concentration of pesticide in inflow to compartment I,	μg/l	User (through subroutine INPUTS)
DC(I)	Derivative of C(I)	μg/l/day	Computed
AF1(I)	Fraction of pesticide in dissolved phase in compartment I		Computed
AF2(I)	Fraction of pesticide in particulate phase in compartment I		Computed
F(I,J)	Net reaction rate of type J in compartment I	1/day	Computed

J	Type
1	Photolysis in dissolved phase
2	Oxidation in dissolved phase
3	Hydrolysis in dissolved phase
4	Volatilization in dissolved phase
5	Biolysis in dissolved phase
6	Settling in particulate phase
7	Oxidation in particulate phase
8	Hydrolysis in particulate phase
9	Biolysis in particulate phase

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(4-78)

```
 COMMON /REAC1/ AQY(30),AKI(30),AKP(30),OXK(30),RO2(30),AKO(30),
1BKB(30),AKA(30),AKN(30),PH(30),AKH(30),AKV(30),GRM(30),YLD(30),
2HKS(30),XMB(30),AKB(30)
```

Variable	Description	Provided by:
AQY(I)	Quantum yield for photolysis in dissolved phase	User
AKI(I)	Summation of the molar extinction coefficient times the light intensity, 1/day	User
AKP(I)	Photolysis rate constant for the dissolved phase = AQY(I)*AKI(I) 1/day	Computed
OXK(I)	Oxidation rate constant for the dissolved phase 1/mole-day	User
RO2(I)	Concentration of RO_2 in the dissolved phase mole/l	User
AKO(I)	Oxidation rate constant in the dissolved phase = OXK(I)*RO2(I)	Computed
BKB(I)	Base catalyzed hydrolysis rate constant in dissolved phase 1/mole-day	User
AKA(I)	Acid catalysed hydrolysis rate constant in dissolved phase 1/mole-day	User
AKN(I)	Neutral hydrolysis rate constant in dissolved phase 1/day	User
PH(I)	Hydrogen ion concentration in dissolved phase (cannot equal zero) mole/l	User
AKH(I)	Hydrolysis rate constant in dissolved phase = BKB(I)*10**(-14)/PH(I) + AKA(I)*PH(I) + AKN(I)	Computed
AKV(I)	Volatilization rate constant in dissolved phase 1/day	User
GRM(I)	Maximum growth of the bugs in the dissolved phase 1/day	User
YLD(I)	Cell yield in the dissolved phase (cannot equal zero) μg/μg	User

(continued on next page)

Variable	Description		Provided by:
HKS(I)	Half saturation concentration in the dissolved phase	μg/l	User
XMB(I)	Concentration of biomass	μg/l	User
AKB(I)	Biolysis rate constant in the dissolved phase = GRM(I)*XMB(I)/YLD(I)/HKS(I)	1/day	Computed

Note: I refers to compartment number

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(4-76)

```
     COMMON /REAC2/ OXKP(30),RO2P(30),AKOP(30),BKBP(30),AKAP(30),AKNP(30),
    1PHP(30),AKHP(30),GRMP(30),YLDP(30),HKSP(30),XMBP(30),AKBP(30)
```

Variable	Description		Provided by:
OXKP(I)	Oxidation rate in the particulate phase	1/mole-day	User
RO2P(I)	Concentration of RO_2 in the particulate phase	mole/l	User
AKOP(I)	Oxidation rate constant in particulate phase = OXKP(I)*RO2P(I)	1/day	Computed
BKBP(I)	Base catalyzed hydrolysis rate constant in particulate phase	1/mole-day	User
AKAP(I)	Acid catalyzed hydrolysis rate constant in particulate phase	1/mole-day	User
AKNP(I)	Neutral hydrolysis rate constant in particulate phase	1/day	User
PHP(I)	Hydrogen ion concentration in particulate phase (cannot equal zero)	mole/l	User
AKHP(I)	Hydrolysis rate constant in particulate phase = BKBP(I)*10**(-14)/PHP(I) + AKAP(I)*PHP(I) + AKNP(I)		Computed
GRMP(I)	Maximum growth rate of bugs in particulate phase	1/day	User
YLDP(I)	Cell yield in particulate phase (cannot equal zero)	g/g	User
HKSP(I)	Half saturation concentration in particulate phase (cannot equal zero)	g/l	User
XMBP(I)	Concentration of biomass in particulate phase	g/l	User
AKBP(I)	Biolysis rate constant in particulate phase = GRMP(I)*XMBP(I)/YLDP(I)/HKSP(I)	1/day	Computed

Note: I refers to compartment number

INSTRUCTIONS FOR RUNNING 'TOXIC'

TOXIC is a 30-compartment model for simulating toxic organics in reservoirs. The data for TOXIC is contained in the file DATA. The file DATA is assigned logical unit #5 in TOXIC (corresponding to PRIME file unit #1).

In order to run TOXIC, the file DATA must first be opened. This is done by the command:

```
O DATA 1 1
```

To run TOXIC, type the command:

```
SEG #TOXIC
```

The output from TOXIC will appear on the terminal. If you wish to store the output in a file, use the COMO command thus:

```
COMO filename

      .

      .

      .

COMO -E
```

Whatever appears on the terminal between the commands COMO filename and COMO -E will be stored in the file specified by filename. This file can then be spooled or edited as desired.

The following example illustrates the procedure just described. The output from TOXIC is stored in the file OUTPUT. (OK is the system prompt).

```
OK,O DATA 1 1

OK,COMO OUTPUT

OK,SEG #TOXIC

        .

        .

Output from TOXIC appears on the terminal
```

BEGIN FIRST LINE OF TEXT HERE
TYPING GUIDE SHEET
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD. BEGIN ALL SECTIONS HERE

```
.
.
OK,COMO -E
```

The file OUTPUT now contains the output from TOXIC. When not required any more, it should be deleted.

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9-1/8"
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BOTTOM OF IMAGE AREA: OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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PROGRAM CODES

6 1/2''

TOXIC
TOXIC - 30 compartment version
TWOCOMP
TWOCOMP1

9 1/8''
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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```
.NULL.
C
      COMMON NUM,H,OUTDEL,TFIN,NERR,NOUT
      COMMON QIN(20),QOUT(20),Q(20,20),IPOS(20,20),DIS(20,20)
      COMMON C(20),DC(20),F(20,10),CIN(20),V(20),AF1(20),AF2(20)
      COMMON AM(20)
C
C
      DIMENSION PC(20),E(20,20),SA(20,20),AL(20,20),HMD(20)
      DIMENSION AQY(20),AKI(20),AKP(20)
      DIMENSION OXK(20),RO2(20),AKO(20),BKB(20)
      DIMENSION AKA(20),AKN(20),PH(20),AKH(20)
      DIMENSION AKV(20),AKS(20)
      DIMENSION GRM(20),YLD(20),HKS(20),XMB(20),AKB(20)
      DIMENSION OXKP(20),RO2P(20),AKOP(20),BKBP(20)
      DIMENSION AKAP(20),AKNP(20),PHP(20),AKHP(20)
      DIMENSION GRMP(20),YLDP(20),HKSP(20),XMBP(20),AKBP(20)
C
C
C
C*****INITIALIZE VARIABLES
C
      DO 100 I=1,20
      QIN(I)=0.0
      QOUT(I)=0.0
      CIN(I)=0.0
      HMD(I)=1.0
      DO 110 J=1,20
      IPOS(I,J)=0
      Q(I,J)=0.0
      E(I,J)=0.0
      SA(I,J)=0.0
      AL(I,J)=1.0
  110 CONTINUE
  100 CONTINUE
C
C*****SET ALL REACTION RATES TO ZERO
C
      DO 120 I=1,20
      AQY(I)=0.0
      AKI(I)=0.0
      OXK(I)=0.0
      RO2(I)=0.0
      BKB(I)=0.0
      AKA(I)=0.0
      AKN(I)=0.0
```

Table 1. TOXIC code in Extended Fortran for PRIME 750 computer

```
      PH(I)=1.0E-07
      AKV(I)=0.0
      GRM(I)=0.0
      XMB(I)=0.0
      YLD(I)=1.0
      HKS(I)=1.0
      AKS(I)=0.0
C
      OXKP(I)=0.0
      RO2P(I)=0.0
      BKBP(I)=0.0
      AKAP(I)=0.0
      AKNP(I)=0.0
      PHP(I)=1.0E-07
      GRMP(I)=0.0
      XMBP(I)=0.0
      YLDP(I)=1.0
      HKSP(I)=1.0
C
  120 CONTINUE
C
C
C*****SET LOGICAL UNIT NUMBERS FOR INPUT AND OUTPUT
C
      INPUT=5
      NOUT=1
      READ(INPUT,200) CHEM
  200 FORMAT(A10)
      WRITE(NOUT,210) CHEM
  210 FORMAT(///1X,'INPUT DATA FOR',1X,A10)
C
      READ(INPUT,*) NUM,H,OUTDEL,TFIN
      WRITE(NOUT,230) NUM,H,OUTDEL,TFIN
  230 FORMAT(1X,'NUMBER OF COMPARTMENTS=',I5/1X,
     1          'STEP SIZE FOR CALCULATIONS=',F10.2,' DAYS',/1X,
     2          'TIME BETWEEN OUTPUT POINTS=',F10.2,' DAYS',/1X,
     3          'TIME FOR SIMULATION       =',F10.2,' DAYS',/)
C
C
      READ(INPUT,*) (V(I),I=1,NUM)
      READ(INPUT,*) (QIN(I),I=1,NUM)
      READ(INPUT,*) (QOUT(I),I=1,NUM)
C
      WRITE(NOUT,260)
  260 FORMAT(//,'COMPARTMENT',5X,'VOLUME,MILLION CU.M',5X,
     1'INFLOW, MILLION CU.M',5X,'OUTFLOW, MILLION CU.M')
      DO 270 I=1,NUM
  270 WRITE(NOUT,280) I,V(I),QIN(I),QOUT(I)
  280 FORMAT(/I6,15X,F8.4,15X,F8.4,15X,F8.4)
C
C
```

```
      DO 281 I=1,NUM
  281 READ(INPUT,*) (Q(I,J),J=1,NUM)
      WRITE(NOUT,285)
  285 FORMAT(/20X,'INTERFLOW MATRIX FOR COMPARTMENTS')
      DO 290 I=1,NUM
  290 WRITE(NOUT,300) (Q(I,J),J=1,NUM)
  300 FORMAT(15(2X,F6.4))
C
C*****CHECK FOR A FLOW BALANCE ON EACH COMPARTMENT
C
      DO 301 I=1,NUM
      FIN=QIN(I)
      FOUT=QOUT(I)
      DO 302 J=1,NUM
      FIN=FIN+Q(J,I)
  302 FOUT=FOUT+Q(I,J)
      IF (FIN.NE.FOUT) CALL ERROR(1,I)
  301 CONTINUE
C
      READ(INPUT,*) (C(I),I=1,NUM)
      READ(INPUT,*) (AM(I),I=1,NUM)
      READ(INPUT,*) (PC(I),I=1,NUM)
      DO 310 I=1,NUM
      AF1(I)=1.0/(1.0 + AM(I)*PC(I))
  310 AF2(I)=1.0 - AF1(I)
C
      WRITE(NOUT,320)
  320 FORMAT(/'COMPARTMENT',5X,'INITIAL',10X,'MASS OF',10X,'PARTITION',
     17X,'FRACTION IN',5X,'FRACTION IN',/12X,'CONCENTRATION',4X'SUSPENDE
     2D SOLIDS',4X,'COEFFICIENT',4X,'DISSOLVED PHASE',1X,'SUSPENDED PHAS
     3E')
C
      DO 330 I=1,NUM
  330 WRITE(NOUT,340) I,C(I),AM(I),PC(I),AF1(I),AF2(I)
  340 FORMAT(I6,10X,F6.4,10X,E9.3,10X,F6.0,2(10X,F5.3))
C
C
      DO 341 I=1,NUM
  341 READ(INPUT,*) (E(I,J),J=1,NUM)
      DO 343 I=1,NUM
  343 READ(INPUT,*) (SA(I,J),J=1,NUM)
      DO 345 I=1,NUM
  345 READ(INPUT,*) (AL(I,J),J=1,NUM)
      READ(INPUT,*) (HMD(I),I=1,NUM)
C
C
      WRITE(NOUT,350)
  350 FORMAT(/23X'DISPERSION COEFFICIENTS')
      WRITE(NOUT,360) ((E(I,J),J=1,NUM),I=1,NUM)
  360 FORMAT(/1X,9E8.1)
      WRITE(NOUT,370)
  370 FORMAT(/25X'INTERFACE AREAS')
      WRITE(NOUT,380) ((SA(I,J),J=1,NUM),I=1,NUM)
  380 FORMAT(/9F8.3)
      WRITE(NOUT,390)
  390 FORMAT(/20X'MEAN LENGTH BETWEEN COMPARTMENTS')
      WRITE(NOUT,400) ((AL(I,J),J=1,NUM),I=1,NUM)
  400 FORMAT(/1X,9E9.3)
C
      DO 402 I=1,NUM
      DO 403 J=1,NUM
  403 DIS(I,J)=(E(I,J)*SA(I,J))/AL(I,J)
  402 CONTINUE
C
C*****READ IN REACTION RATES
C
      READ(INPUT,*) (AQY(I),I=1,NUM)
C
      READ(INPUT,*) (AKI(I),I=1,NUM)
C
      DO 430 I=1,NUM
      AKP(I)=AQY(I)*AKI(I)
  430 CONTINUE
C
C*****AKP IS THE PHOTOLYSIS RATE CONSTANT (PER DAY)
C
      DO 440 I=1,NUM
  440 F(I,1)=AF1(I)*AKP(I)
C
C*****OXIDATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (OXK(I),I=1,NUM)
C
      READ(INPUT,*) (RO2(I),I=1,NUM)
C
      DO 470 I=1,NUM
  470 AKO(I)=OXK(I)*RO2(I)
C
C*****AKO IS THE OXIDATION RATE CONSTANT (PER DAY)
C
      DO 480 I=1,NUM
  480 F(I,2)=AF1(I)*AKO(I)
C
      READ(INPUT,*) (BKB(I),I=1,NUM)
C
      READ(INPUT,*) (AKA(I),I=1,NUM)
C
      READ(INPUT,*) (AKN(I),I=1,NUM)
C
      READ(INPUT,*) (PH(I),I=1,NUM)
```

```
C
      DO 500 I=1,NUM
  500 AKH(I)=BKB(I)*10**(-14)/PH(I) + AKA(I)*PH(I) + AKN(I)
C
      DO 510 I=1,NUM
  510 F(I,3)=AF1(I)*AKH(I)
C
C*****VOLATILIZATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (AKV(I),I=1,NUM)
C
      DO 520 I=1,NUM
  520 F(I,4)=AF1(I)*AKV(I)
C
C*****BIODEGRADATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (GRM(I),I=1,NUM)
C
      READ(INPUT,*) (YLD(I),I=1,NUM)
C
      READ(INPUT,*) (HKS(I),I=1,NUM)
C
      READ(INPUT,*) (XMB(I),I=1,NUM)
C
      DO 540 I=1,NUM
  540 AKB(I)=GRM(I)*XMB(I)/YLD(I)/HKS(I)
C
      DO 550 I=1,NUM
  550 F(I,5)=AF1(I)*AKB(I)
C
C*****SETTLING FOR THE PARTICULATE PHASE
C
      READ(INPUT,*) (AKS(I),I=1,NUM)
      WRITE(NOUT,562) (AKS(I),I=1,NUM)
  562 FORMAT(/21X,'SETTLING RATE CONSTANTS',//1X,10(1X,F6.2))
C
      DO 560 I=1,NUM
  560 F(I,6)=AF2(I)*AKS(I)
C
C*****POSITION OF COMPARTMENT WITH RESPECT TO OTHERS
C
      DO 580 I=1,NUM
  580 READ(INPUT,*) (IPOS(I,J),J=1,NUM)
C
      WRITE(NOUT,585)
  585 FORMAT(//20X,'COMPARTMENT POSITION MATRIX')
      WRITE(NOUT,590) ((IPOS(I,J),J=1,NUM),I=1,NUM)
  590 FORMAT(14X,9I4)
```

```
C
C*****
C*********************************
C***** REACTION RATES FOR THE *****
C***** PARTICULATE PHASE      *****
C*********************************
C*****
C
C*****OXIDATION
C
      READ(INPUT,*) (OXKP(I),I=1,NUM)
C
      READ(INPUT,*) (RO2P(I),I=1,NUM)
C
      DO 600 I=1,NUM
  600 AKOP(I)=OXKP(I)*RO2P(I)
C
      DO 610 I=1,NUM
  610 F(I,7)=AF2(I)*AKOP(I)
C
C*****HYDROLYSIS
C
      READ(INPUT,*) (BKBP(I),I=1,NUM)
C
      READ(INPUT,*) (AKAP(I),I=1,NUM)
C
      READ(INPUT,*) (AKNP(I),I=1,NUM)
      READ(INPUT,*) (PHP(I),I=1,NUM)
C
      DO 620 I=1,NUM
  620 AKHP(I)=BKBP(I)*10**(-14)/PHP(I) + AKAP(I)*PHP(I) + AKNP(I)
C
      DO 630 I=1,NUM
  630 F(I,8)=AF2(I)*AKHP(I)
C
C*****BIODEGRADATION
C
      READ(INPUT,*) (GRMP(I),I=1,NUM)
      READ(INPUT,*) (YLDP(I),I=1,NUM)
      READ(INPUT,*) (HKSP(I),I=1,NUM)
      READ(INPUT,*) (XMBP(I),I=1,NUM)
C
      DO 640 I=1,NUM
  640 AKBP(I)=GRMP(I)*XMBP(I)/YLDP(I)/HKSP(I)
C
      DO 650 I=1,NUM
  650 F(I,9)=AF2(I)*AKBP(I)
C
C*****PRINT REACTION RATES FOR DISSOLVED AND PARTICULATE PHASE
C
```

```
      WRITE(NOUT,680)
  680 FORMAT(//11X,'PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)'/
     121X,'IN THE DISSOLVED PHASE')
      WRITE(NOUT,685)
  685 FORMAT(//3X,'CMPN',2X,'PHOTOLYSIS  OXIDATION  HYDROLYSIS   BIOLYSI
     1S  VOLATILIZATION')
      DO 690 I=1,NUM
  690 WRITE(NOUT,700) I,AKP(I),AKO(I),AKH(I),AKB(I),AKV(I)
  700 FORMAT(1X,I5,5F12.7)
C
      WRITE(NOUT,710)
  710 FORMAT(//11X,'PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)'/
     120X,'IN THE PARTICULATE PHASE')
      WRITE(NOUT,720)
  720 FORMAT(//13X,'CMPN',2X,'OXIDATION  HYDROLYSIS   BIOLYSIS')
      DO 730 I=1,NUM
  730 WRITE(NOUT,740) I,AKOP(I),AKHP(I),AKBP(I)
  740 FORMAT(11X,I5,3F12.7)
C
C*****CHECK FOR INPUT ERRORS
C
      IF (NERR.EQ.0) GO TO 800
C
      WRITE(NOUT,750) NERR
  750 FORMAT(//1X,I3,' ERRORS FOUND IN INPUT DATA - SIMULATION NOT ATTEM
     1PTED')
      CALL EXIT
C
  800 CALL SOLVE
C
      CALL EXIT
      END
      SUBROUTINE ERROR(K,I)
      NERR=NERR+1
      GO TO (100,200),K
  100 WRITE(1,110) I
  110 FORMAT(/'***ERROR*** FLOWS FOR COMPARTMENT',I3,' DO NOT BALANCE')
      RETURN
  200 RETURN
      END
      SUBROUTINE SOLVE
C
      COMMON NUM,H,OUTDEL,TFIN,NERR,NOUT
      COMMON QIN(20),QOUT(20),Q(20,20),IPOS(20,20),DIS(20,20)
      COMMON C(20),DC(20),F(20,10),CIN(20),V(20),AF1(20),AF2(20)
      COMMON AM(20)
C
C
      DIMENSION TOUT(50),CL(20),A1(20),A2(20),A3(20),A4(20)
      DIMENSION CT(50,20),CD(50,20),CP(50,20),CM(50,20)
      DIMENSION R1(20),R2(20),R3(20),R4(20),R5(20)
      DIMENSION EXT(20),FNET(20)
```

```
C
      WRITE(1,111)
  111 FORMAT(//20X,'R1  = FLUX DUE TO INFLOW FROM OTHER COMPARTMENTS',
     1//20X,'R2  = FLUX DUE TO OUTFLOW TO  OTHER COMPARTMENTS',
     2//20X,'R3  = FLUX DUE TO REACTION',
     3//20X,'R4  = FLUX DUE TO DISPERSION (NET INFLOW)',
     4//20X,'R5  = FLUX DUE TO SETTLING FROM ABOVE',
     5//20X,'EXT = FLUX DUE FLOWS TO OR FROM OUTSIDE THE SYSTEM',
     6//20X,'FNET= NET FLUX TO EACH COMPARTMENT')
      WRITE(1,222)
  222 FORMAT(//20X,'ALL UNITS IN KG/DAY')
      TIM=0.0
      DTHLF=0.5*H
      TSAV=OUTDEL
      DO 40 I=1,NUM
      TOUT(1)=TIM
      CT(1,I)=C(I)
      CD(1,I)=AF1(I)*C(I)
      CP(1,I)=AF2(I)*C(I)
      CM(1,I)=CP(1,I)/AM(I)
   40 CONTINUE
      IOUT=2
   50 DO 100 I=1,NUM
  100 CL(I)=C(I)
C
C*****SET INPUT CONCENTRATION FOR THE FIRST COMPARTMENT
C
      CIN(1)=0.05*EXP(-0.00045*TIM)
C
      CALL DIFFEQ(R1,R2,R3,R4,R5,EXT,FNET)
      DO 110 I=1,NUM
      A1(I)=DC(I)
  110 C(I)=CL(I)+DTHLF*A1(I)
      CALL DIFFEQ(R1,R2,R3,R4,R5,EXT,FNET)
      DO 120 I=1,NUM
      A2(I)=DC(I)
  120 C(I)=CL(I)+DTHLF*A2(I)
      CALL DIFFEQ(R1,R2,R3,R4,R5,EXT,FNET)
      DO 130 I=1,NUM
      A3(I)=DC(I)
  130 C(I)=CL(I)+H*A3(I)
      CALL DIFFEQ(R1,R2,R3,R4,R5,EXT,FNET)
      DO 140 I=1,NUM
      A4(I)=DC(I)
  140 C(I)=CL(I)+H*(A1(I)+2.*A2(I)+2.*A3(I)+A4(I))/6.
C
      TIM=TIM+H
      TNEX=AMINO(TSAV,TFIN)
      IF(TIM.GE.TNEX) GO TO 150
      GO TO 50
  150 DO 160 I=1,NUM
```

```
      TOUT(IOUT)=TIM
      CT(IOUT,I)=C(I)
      CD(IOUT,I)=AF1(I)*C(I)
      CP(IOUT,I)=AF2(I)*C(I)
      CM(IOUT,I)=CP(IOUT,I)/AM(I)
  160 CONTINUE
C
      WRITE(1,401) TIM
  401 FORMAT(///30X,'TIME=',F8.1//'CMPN',5X,'R1',14X,'R2',14X,
     1'R3',13X,'R4',13X,'R5',12X,'EXT',12X,'FNET'/)
      DO 402 I=1,NUM
  402 WRITE(1,403) I,R1(I),R2(I),R3(I),R4(I),R5(I),EXT(I),FNET(I)
  403 FORMAT(I3,7(3X,E12.6))
      IF(TIM.GE.TFIN) GO TO 170
      IOUT=IOUT+1
      TSAV=TSAV+OUTDEL
      GO TO 50
C
  170 WRITE(NOUT,180) TFIN
  180 FORMAT(//17X'SIMULATION HALTED AT TIME = ',F7.1)
C
C*****PRINT RESULTS
C
      WRITE(NOUT,200)
  200 FORMAT(///10X,'TOTAL CONCENTRATION OF PESTICIDE OVER TIME (PPB)'
     1//1X,'TIME(DAYS)',15X,'COMPARTMENT NUMBER')
      WRITE(NOUT,205) (I,I=1,NUM)
  205 FORMAT(/,9X,9I7/)
      DO 210 L=1,IOUT
  210 WRITE(NOUT,220) TOUT(L),(CT(L,I),I=1,NUM)
  220 FORMAT(1X,F10.1,9F7.4)
C
      WRITE(NOUT,230)
  230 FORMAT(///10X,'DISSOLVED CONCENTRATION OF PESTICIDE OVER TIME
     1(PPB)'//1X,'TIME(DAYS)',15X,'COMPARTMENT NUMBER')
      WRITE(NOUT,205) (I,I=1,9)
      DO 240 L=1,IOUT
  240 WRITE(NOUT,220) TOUT(L),(CD(L,I),I=1,NUM)
C
      WRITE(NOUT,260)
  260 FORMAT(///10X,'PARTICULATE CONCENTRATION OF PESTICIDE OVER TIME
     1(PPB)',//1X,'TIME(DAYS)',15X,'COMPARTMENT NUMBER'/)
      WRITE(NOUT,205) (I,I=1,9)
      DO 270 L=1,IOUT
  270 WRITE(NOUT,220) TOUT(L),(CP(L,I),I=1,NUM)
C
```

```
      WRITE(NOUT,280)
  280 FORMAT(///10X,'MASS OF PESTICIDE ON THE MASS OF SOLIDS  (MICROGRAM
     1 PER KILOGRAM)'///1X,'TIME(DAYS)',15X,'COMPARTMENT NUMBER')
      DO 290 L=1,IOUT
  290 WRITE(NOUT,300) TOUT(L),(CM(L,I),I=1,NUM)
  300 FORMAT(1X,F8.1,9(1X,F7.2))
C
      RETURN
      END
C
      SUBROUTINE DIFFEQ(R1,R2,R3,R4,R5,EXT,FNET)
C
C
      COMMON NUM,H,OUTDEL,TFIN,NERR,NOUT
      COMMON QIN(20),QOUT(20),Q(20,20),IPOS(20,20),DIS(20,20)
      COMMON C(20),DC(20),F(20,10),CIN(20),V(20),AF1(20),AF2(20)
      COMMON AM(20)
C
      DIMENSION R1(20),R2(20),R3(20),R4(20),R5(20)
      DIMENSION EXT(20),FNET(20)
C
C
      DO 100 I=1,NUM
C
C*****INITIALIZE NET FLUXES
C
      R1(I)=0.0
      R2(I)=0.0
      R3(I)=0.0
      R4(I)=0.0
      R5(I)=0.0
C
C*****MASS FLUX DUE TO INFLOWS FROM OTHER COMPARTMENTS
C
      DO 110 J=1,NUM
  110 R1(I)=R1(I)+Q(J,I)*C(J)
C
C*****MASS FLUX DUE TO OUTFLOWS TO OTHER COMPARTMENTS
C
      DO 120 J=1,NUM
  120 R2(I)=R2(I)+Q(I,J)*C(I)
C
C******CHANGE IN CONCENTRATION DUE TO REACTION
C
```

```
      DO 130 K=1,9
  130 R3(I)=R3(I)+F(I,K)*C(I)*V(I)
C
C*****MASS FLUX DUE TO DISPERSION
C
      DO 140 J=1,NUM
  140 R4(I)=R4(I)+DIS(I,J)*(C(J)-C(I))
C
C*****MASS FLUX DUE TO SETTLING FROM ABOVE
C
      DO 150 J=1,NUM
  150 R5(I)=R5(I)+F(J,6)*C(J)*IPOS(J,I)*V(J)
C
C*****SET UP DIFFERENTIAL EQUATION FOR EACH COMPARTMENT
C
      EXT(I)=QIN(I)*CIN(I) - QOUT(I)*C(I)
      FNET(I)=EXT(I) + R1(I) - R2(I) - R3(I) + R4(I) + R5(I)
      DC(I)=FNET(I)/V(I)
C
  100 CONTINUE
      RETURN
      END
BOTTOM
Q
```

TYPING GUIDE SHEET
EPA-287 (Cin.)
(4-78)

```
.NULL.
C
C*****PROGRAM FOR PESTICIDE SIMULATION IN AQUATIC SYSTEMS
C*****30 COMPARTMENT MODEL
C*****AUTHOR : NARASINGA B. RAO
C
      COMMON /GEN/ NUM,H,OUTDEL,TIM,TFIN,NERR,NOUT,INTER
      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30)
     1,IPOS(30,30),ED(30,30),EP(30,30),SA(30,30),AL(30,30)
     2,DISD(30,30),DISP(30,30)
      COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30),PC(30)
      COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
C
      INTEGER*4 CHEM(3)
      COMMON /REAC1/ AQY(30),AKI(30),AKP(30),OXK(30),RO2(30),AKO(30),
     1BKB(30),AKA(30),AKN(30),PH(30),AKH(30),AKV(30),GRM(30),YLD(30),
     2HKS(30),XMB(30),AKB(30)
      COMMON /REAC2/ OXKP(30),RO2P(30),AKOP(30),BKBP(30),AKAP(30),
     1AKNP(30),PHP(30),AKHP(30),GRMP(30),YLDP(30),HKSP(30),XMBP(30),
     2AKBP(30)
C
C*****INITIALIZE VARIABLES
C
      DO 100 I=1,30
      QIN(I)=0.0
      QOUT(I)=0.0
      CIN(I)=0.0
      DO 110 J=1,30
      IPOS(I,J)=0
      Q(I,J)=0.0
      ED(I,J)=0.0
      EP(I,J)=0.0
      SA(I,J)=0.0
      AL(I,J)=1.0
  110 CONTINUE
  100 CONTINUE
C
C*****SET ALL REACTION RATES TO ZERO
C
      DO 120 I=1,30
      AQY(I)=0.0
      AKI(I)=0.0
      OXK(I)=0.0
      RO2(I)=1.0
      BKB(I)=0.0
      AKA(I)=0.0
```

Table 2. 30 - compartment TOXIC code in Extended Fortran for PRIME 750 computer

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```
      AKN(I)=0.0
      PH(I)=1.0E-07
      AKV(I)=0.0
      GRM(I)=0.0
      XMB(I)=0.0
      YLD(I)=1.0
      HKS(I)=1.0
      AKS(I)=0.0
C
      OXKP(I)=0.0
      RO2P(I)=1.0
      BKBP(I)=0.0
      AKAP(I)=0.0
      AKNP(I)=0.0
      PHP(I)=1.0E-07
      GRMP(I)=0.0
      XMBP(I)=0.0
      YLDP(I)=1.0
      HKSP(I)=1.0
C
  120 CONTINUE
C
      NERR=0
C
C*****SET LOGICAL UNIT NUMBERS FOR INPUT AND OUTPUT
C
      INPUT=5
      NOUT=1
      READ(INPUT,200) CHEM
  200 FORMAT(3A4)
      WRITE(NOUT,210) CHEM
  210 FORMAT(///1X,'INPUT DATA FOR',1X,3A4)
C
      READ(INPUT,*) NUM,H,OUTDEL,TFIN
      WRITE(NOUT,230) NUM,H,OUTDEL,TFIN
  230 FORMAT(1X,'NUMBER OF COMPARTMENTS=',I5/1X,
     1           'STEP SIZE FOR CALCULATIONS=',F10.2,' DAYS',/1X,
     2           'TIME BETWEEN OUTPUT POINTS=',F10.2,' DAYS',/1X,
     3           'TIME FOR SIMULATION       =',F10.2,' DAYS',/)
C
      READ(INPUT,*) (V(I),I=1,NUM)
      READ(INPUT,*) (QIN(I),I=1,NUM)
      READ(INPUT,*) (QOUT(I),I=1,NUM)
C
      DO 281 I=1,NUM
  281 READ(INPUT,*) (Q(I,J),J=1,NUM)
C
C*****CHECK FOR A FLOW BALANCE ON EACH COMPARTMENT
C
      DO 301 I=1,NUM
      FIN=QIN(I)
      FOUT=QOUT(I)
      DO 302 J=1,NUM
      FIN=FIN+Q(J,I)
  302 FOUT=FOUT+Q(I,J)
C
      DIFF=ABS(FIN-FOUT)
      TOL=0.05*FIN
C
      IF (DIFF.GT.TOL) CALL ERROR(1,I)
  301 CONTINUE
C
      READ(INPUT,*) (C(I),I=1,NUM)
      READ(INPUT,*) (AM(I),I=1,NUM)
      READ(INPUT,*) (PC(I),I=1,NUM)
      DO 310 I=1,NUM
      AF1(I)=1.0/(1.0 + AM(I)*PC(I))
  310 AF2(I)=1.0 - AF1(I)
C
      WRITE(NOUT,320)
  320 FORMAT(/'COMPARTMENT',5X,'INITIAL',10X,'MASS OF',10X,'PARTITION',
     17X,'FRACTION IN',5X,'FRACTION IN',/12X,'CONCENTRATION',4X'SUSPENDE
     2D SOLIDS',4X,'COEFFICIENT',4X,'DISSOLVED PHASE',1X,'SUSPENDED PHAS
     3E')
C
      DO 330 I=1,NUM
  330 WRITE(NOUT,340) I,C(I),AM(I),PC(I),AF1(I),AF2(I)
  340 FORMAT(I6,10X,F6.4,10X,E9.3,10X,F6.0,2(10X,F5.3))
C
      NUML=NUM-1
C
      DO 341 I=1,NUML
      II=I+1
  341 READ(INPUT,*) (EP(I,J),J=II,NUM)
      DO 342 I=1,NUML
      II=I+1
  342 READ(INPUT,*) (ED(I,J),J=II,NUM)
      DO 343 I=1,NUML
      II=I+1
  343 READ(INPUT,*) (SA(I,J),J=II,NUM)
      DO 344 I=1,NUML
      II=I+1
  344 READ(INPUT,*) (AL(I,J),J=II,NUM)
C
      DO 345 I=1,NUML
      II=I+1
      DO 345 J=II,NUM
      ED(J,I)=ED(I,J)
      EP(J,I)=ED(I,J)
      SA(J,I)=SA(I,J)
  345 AL(J,I) = AL(I,J)
C
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD (BEGIN SECTIONS) HERE
BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
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```
      DO 402 I=1,NUM
      DO 403 J=1,NUM
      DISD(I,J)=(ED(I,J)*SA(I,J))/AL(I,J)
  403 DISP(I,J)=(EP(I,J)*SA(I,J))/AL(I,J)
  402 CONTINUE
C
C*****READ IN REACTION RATES
C
      READ(INPUT,*) (AQY(I),I=1,NUM)
C
      READ(INPUT,*) (AKI(I),I=1,NUM)
C
      DO 430 I=1,NUM
      AKP(I)=AQY(I)*AKI(I)
  430 CONTINUE
C
C*****AKP IS THE PHOTOLYSIS RATE CONSTANT (PER DAY)
C
      DO 440 I=1,NUM
  440 F(I,1)=AF1(I)*AKP(I)
C
C*****OXIDATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (OXK(I),I=1,NUM)
C
      READ(INPUT,*) (RO2(I),I=1,NUM)
C
      DO 470 I=1,NUM
  470 AKO(I)=OXK(I)*RO2(I)
C
C*****AKO IS THE OXIDATION RATE CONSTANT (PER DAY)
C
      DO 480 I=1,NUM
  480 F(I,2)=AF1(I)*AKO(I)
C
      READ(INPUT,*) (BKB(I),I=1,NUM)
C
      READ(INPUT,*) (AKA(I),I=1,NUM)
C
      READ(INPUT,*) (AKN(I),I=1,NUM)
C
      READ(INPUT,*) (PH(I),I=1,NUM)
C
      DO 500 I=1,NUM
  500 AKH(I)=BKB(I)*10**(-14)/PH(I) + AKA(I)*PH(I) + AKN(I)
C
      DO 510 I=1,NUM
  510 F(I,3)=AF1(I)*AKH(I)
C
C*****VOLATILIZATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (AKV(I),I=1,NUM)
```

```
C
      DO 520 I=1,NUM
  520 F(I,4)=AF1(I)*AKV(I)
C
C*****BIODEGRADATION FOR THE DISSOLVED PHASE
C
      READ(INPUT,*) (GRM(I),I=1,NUM)
C
      READ(INPUT,*) (YLD(I),I=1,NUM)
C
      READ(INPUT,*) (HKS(I),I=1,NUM)
C
      READ(INPUT,*) (XMB(I),I=1,NUM)
C
      DO 540 I=1,NUM
  540 AKB(I)=GRM(I)*XMB(I)/YLD(I)/HKS(I)
C
      DO 550 I=1,NUM
  550 F(I,5)=AF1(I)*AKB(I)
C
C*****SETTLING FOR THE PARTICULATE PHASE
C
      READ(INPUT,*) (AKS(I),I=1,NUM)
C
      DO 560 I=1,NUM
  560 F(I,6)=AF2(I)*AKS(I)
C
C*****POSITION OF COMPARTMENT WITH RESPECT TO OTHERS
C
      DO 580 I=1,NUM
  580 READ(INPUT,*) (IPOS(I,J),J=1,NUM)
C
C
C*****
C**********************************
C***** REACTION RATES FOR THE *****
C***** PARTICULATE PHASE      *****
C**********************************
C*****
C
C*****OXIDATION
C
      READ(INPUT,*) (OXKP(I),I=1,NUM)
C
      READ(INPUT,*) (RO2P(I),I=1,NUM)
C
      DO 600 I=1,NUM
  600 AKOP(I)=OXKP(I)*RO2P(I)
C
      DO 610 I=1,NUM
  610 F(I,7)=AF2(I)*AKOP(I)
```

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```
C
C*****HYDROLYSIS
C
      READ(INPUT,*) (BKBP(I),I=1,NUM)
C
      READ(INPUT,*) (AKAP(I),I=1,NUM)
C
      READ(INPUT,*) (AKNP(I),I=1,NUM)
      READ(INPUT,*) (PHP(I),I=1,NUM)
C
      DO 620 I=1,NUM
  620 AKHP(I)=BKBP(I)*10**(-14)/PHP(I) + AKAP(I)*PHP(I) + AKNP(I)
C
      DO 630 I=1,NUM
  630 F(I,8)=AF2(I)*AKHP(I)
C
C*****BIODEGRADATION
C
      READ(INPUT,*) (GRMP(I),I=1,NUM)
      READ(INPUT,*) (YLDP(I),I=1,NUM)
      READ(INPUT,*) (HKSP(I),I=1,NUM)
      READ(INPUT,*) (XMBP(I),I=1,NUM)
C
      DO 640 I=1,NUM
  640 AKBP(I)=GRMP(I)*XMBP(I)/YLDP(I)/HKSP(I)
C
      DO 650 I=1,NUM
  650 F(I,9)=AF2(I)*AKBP(I)
C
C*****PRINT REACTION RATES FOR DISSOLVED AND PARTICULATE PHASE
C
      WRITE(NOUT,680)
  680 FORMAT(//11X,'PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)'/
     121X,'IN THE DISSOLVED PHASE')
      WRITE(NOUT,685)
  685 FORMAT(//3X,'CMPN',2X,'PHOTOLYSIS  OXIDATION  HYDROLYSIS   BIOLYSI
     1S  VOLATILIZATION')
      DO 690 I=1,NUM
  690 WRITE(NOUT,700) I,AKP(I),AKO(I),AKH(I),AKB(I),AKV(I)
  700 FORMAT(1X,I5,5F12.7)
C
      WRITE(NOUT,710)
  710 FORMAT(//11X,'PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)'/
     120X,'IN THE PARTICULATE PHASE')
      WRITE(NOUT,720)
  720 FORMAT(//13X,'CMPN',2X,'OXIDATION  HYDROLYSIS   BIOLYSIS')
      DO 730 I=1,NUM
  730 WRITE(NOUT,740) I,AKOP(I),AKHP(I),AKBP(I)
  740 FORMAT(11X,I5,3F12.7)
```

```
C
C*****CHECK FOR INPUT ERRORS
C
      IF (NERR.EQ.0) GO TO 800
C
      WRITE(NOUT,750) NERR
  750 FORMAT(//1X,I3,' ERRORS FOUND IN INPUT DATA - SIMULATION NOT ATTEM
     1PTED')
      GO TO 999
C
C
  800 CONTINUE
      WRITE(NOUT,810)
  810 FORMAT(/1X,'DO YOU WANT AN ECHO CHECK OF THE INPUT DATA?',1X,
     1'(1=YES,2=NO)')
      READ(1,*) IECHO
      IF(IECHO.EQ.1) CALL PRINT
C
      WRITE(NOUT,820)
  820 FORMAT(/'DO YOU WANT INTERMEDIATE OUTPUT (1=YES),(2=NO) ?')
      READ(1,*) INTER
      CALL SOLVE
C
  999 CALL EXIT
      END
C
      SUBROUTINE PRINT
C
      COMMON /GEN/ NUM,H,OUTDEL,TIM,TFIN,NERR,NOUT,INTER
      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30)
     1,IPOS(30,30),ED(30,30),EP(30,30),SA(30,30),AL(30,30)
     2,DISD(30,30),DISP(30,30)
      COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30),PC(30)
      COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
C
      INTEGER*4 CHEM(3)
      COMMON /REAC1/ AQY(30),AKI(30),AKP(30),OXK(30),RO2(30),AKO(30),
     1BKB(30),AKA(30),AKN(30),PH(30),AKH(30),AKV(30),GRM(30),YLD(30),
     2HKS(30),XMB(30),AKB(30)
      COMMON /REAC2/ OXKP(30),RO2P(30),AKOP(30),BKBP(30),AKAP(30),
     1AKNP(30),PHP(30),AKHP(30),GRMP(30),YLDP(30),HKSP(30),XMBP(30),
     2AKBP(30)
      WRITE(NOUT,260)
  260 FORMAT(//,'COMPARTMENT',5X,'VOLUME,MILLION CU.M',5X,
     1'INFLOW, MILLION CU.M',5X,'OUTFLOW, MILLION CU.M')
      DO 270 I=1,NUM
  270 WRITE(NOUT,280) I,V(I),QIN(I),QOUT(I)
  280 FORMAT(/I6,15X,F8.4,15X,F8.4,15X,F8.4)
C
```

```
      WRITE(NOUT,285)
  285 FORMAT(/20X,'INTERFLOW MATRIX FOR COMPARTMENTS')
      DO 290 I=1,NUM
      WRITE(NOUT,283) I
  283 FORMAT(/20X,'COMPARTMENT',I5/)
  290 WRITE(NOUT,300) (Q(I,J),J=1,NUM)
  300 FORMAT(5(2X,E12.5))
C
      WRITE(NOUT,350)
  350 FORMAT(/9X'DISPERSION COEFFICIENTS FOR DISSOLVED PHASE')
      DO 4001 I=1,NUM
      WRITE(NOUT,283) I
 4001 WRITE(NOUT,300) (ED(I,J),J=1,NUM)
      WRITE(NOUT,4005)
 4005 FORMAT(/9X'DISPERSION COEFFICIENTS FOR PARTICULATE PHASE')
      DO 4010 I=1,NUM
      WRITE(NOUT,283) I
 4010 WRITE(NOUT,300) (EP(I,J),J=1,NUM)
      WRITE(NOUT,370)
  370 FORMAT(/25X'INTERFACE AREAS')
      DO 4002 I=1,NUM
      WRITE(NOUT,283) I
 4002 WRITE(NOUT,300) (SA(I,J),J=1,NUM)
      WRITE(NOUT,390)
  390 FORMAT(/20X'MEAN LENGTH BETWEEN COMPARTMENTS')
      DO 4003 I=1,NUM
      WRITE(NOUT,283) I
 4003 WRITE(NOUT,300) (AL(I,J),J=1,NUM)
C
      WRITE(NOUT,562) (AKS(I),I=1,NUM)
  562 FORMAT(/21X,'SETTLING RATE CONSTANTS',//1X,10(1X,F6.2))
      WRITE(NOUT,585)
  585 FORMAT(//20X,'COMPARTMENT POSITION MATRIX')
      DO 600 I=1,NUM
  600 WRITE(NOUT,610) (IPOS(I,J),J=1,NUM)
  610 FORMAT(10X,30I2)
C
      RETURN
      END
C
      SUBROUTINE ERROR(K,I)
      NERR=NERR+1
      GO TO (100,200),K
  100 WRITE(1,110) I
  110 FORMAT(/'***ERROR*** FLOWS FOR COMPARTMENT',I3,' DO NOT BALANCE')
      RETURN
  200 RETURN
      END
C
      SUBROUTINE SOLVE
C
```

```
      COMMON /GEN/ NUM,H,OUTDEL,TIM,TFIN,NERR,NOUT,INTER
      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30)
     1,IPOS(30,30),ED(30,30),EP(30,30),SA(30,30),AL(30,30)
     2,DISD(30,30),DISP(30,30)
      COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30)
      COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
      COMMON /FLUX/ R1(30),R2(30),R3(30),R4(30),R5(30),EXT(30),FNET(30)
C
C
      DIMENSION TOUT(50),CL(30),A1(30),A2(30),A3(30),A4(30)
      DIMENSION CT(50,30),CD(50,30),CP(50,30),CM(50,30)
C
      IF(INTER.GT.1) GO TO 223
C
      WRITE(1,111)
  111 FORMAT(//20X,'R1  = FLUX DUE TO INFLOW FROM OTHER COMPARTMENTS',
     1//20X,'R2  = FLUX DUE TO OUTFLOW TO  OTHER COMPARTMENTS',
     2//20X,'R3  = FLUX DUE TO REACTION',
     3//20X,'R4  = FLUX DUE TO DISPERSION (NET INFLOW)',
     4//20X,'R5  = FLUX DUE TO SETTLING FROM ABOVE',
     5//20X,'EXT = FLUX DUE FLOWS TO OR FROM OUTSIDE THE SYSTEM',
     6//20X,'FNET= NET FLUX TO EACH COMPARTMENT')
      WRITE(1,222)
  222 FORMAT(//20X,'ALL UNITS IN KG/DAY')
C
  223 CONTINUE
      TIM=0.0
      DTHLF=0.5*H
      TSAV=OUTDEL
      DO 40 I=1,NUM
      TOUT(1)=TIM
      CT(1,I)=C(I)
      CD(1,I)=AF1(I)*C(I)
      CP(1,I)=AF2(I)*C(I)
      CM(1,I)=CP(1,I)/AM(I)
   40 CONTINUE
      IOUT=2
   50 DO 100 I=1,NUM
  100 CL(I)=C(I)
C
C*****SET INPUT CONCENTRATIONS FOR COMPARTMENTS
C
      CALL INPUTS
C
      CALL DIFFEQ
      DO 110 I=1,NUM
      A1(I)=DC(I)
  110 C(I)=CL(I)+DTHLF*A1(I)
      CALL DIFFEQ
      DO 120 I=1,NUM
      A2(I)=DC(I)
  120 C(I)=CL(I)+DTHLF*A2(I)
```

```
      CALL DIFFEQ
      DO 130 I=1,NUM
      A3(I)=DC(I)
  130 C(I)=CL(I)+H*A3(I)
      CALL DIFFEQ
      DO 140 I=1,NUM
      A4(I)=DC(I)
  140 C(I)=CL(I)+H*(A1(I)+2.*A2(I)+2.*A3(I)+A4(I))/6.
C
      TIM=TIM+H
      TNEX=AMINO(TSAV,TFIN)
      IF(TIM.GE.TNEX) GO TO 150
      GO TO 50
  150 DO 160 I=1,NUM
      TOUT(IOUT)=TIM
      CT(IOUT,I)=C(I)
      CD(IOUT,I)=AF1(I)*C(I)
      CP(IOUT,I)=AF2(I)*C(I)
      CM(IOUT,I)=CP(IOUT,I)/AM(I)
  160 CONTINUE
C
      WRITE(NOUT,1610) TIM
 1610 FORMAT(///20X,'TIME=',F7.1,' DAYS'//)
      WRITE(NOUT,1602) (C(I),I=1,NUM)
 1602 FORMAT(5(2X,E12.5))
C
      WRITE(NOUT,1603) V(16),AL(16,1)
 1603 FORMAT(/10X,'VOL=',F10.2,10X,'AL=',F10.3,//)
C
      IF(INTER.GT.1) GO TO 444
      WRITE(1,401) TIM
  401 FORMAT(///30X,'TIME=',F8.1//'CMPN',5X,'R1',14X,'R2',14X,
     1'R3',13X,'R4',13X,'R5',12X,'EXT',12X,'FNET'/)
      DO 402 I=1,NUM
  402 WRITE(1,403) I,R1(I),R2(I),R3(I),R4(I),R5(I),EXT(I),FNET(I)
  403 FORMAT(I3,7(3X,E12.6))
C
  444 CONTINUE
      IF(TIM.GE.TFIN) GO TO 170
      IOUT=IOUT+1
      TSAV=TSAV+OUTDEL
      GO TO 50
C
  170 WRITE(NOUT,190) TFIN
  180 FORMAT(//17X'SIMULATION HALTED AT TIME = ',F7.1)
C
C*****PRINT RESULTS
C
      WRITE(NOUT,200)
  200 FORMAT(///10X,'TOTAL CONCENTRATION OF PESTICIDE OVER TIME (PPB)'
     1//26X,'COMPARTMENT NUMBER'//)
```

```
      WRITE(NOUT,205) (I,I=1,NUM)
  205 FORMAT(7X,I2,12X,I2,12X,I2,12X,I2,12X,I2)
      DO 210 L=1,IOUT
      WRITE(NOUT,220) TOUT(L)
  220 FORMAT(//23X,'TIME=',F7.1,' DAYS'//)
      WRITE(NOUT,2201) (CT(L,I),I=1,NUM)
 2201 FORMAT(5(2X,E12.5))
  210 CONTINUE
C
      WRITE(NOUT,230)
  230 FORMAT(///10X,'DISSOLVED CONCENTRATION OF PESTICIDE OVER TIME
     1(PPB)'//26X,'COMPARTMENT NUMBER'//)
      WRITE(NOUT,205) (I,I=1,NUM)
      DO 240 L=1,IOUT
      WRITE(NOUT,220) TOUT(L)
  240 WRITE(NOUT,2201) (CD(L,I),I=1,NUM)
C
      WRITE(NOUT,260)
  260 FORMAT(///10X,'PARTICULATE CONCENTRATION OF PESTICIDE OVER TIME
     1(PPB)',//26X,'COMPARTMENT NUMBER'//)
      WRITE(NOUT,205) (I,I=1,NUM)
      DO 270 L=1,IOUT
      WRITE(NOUT,220) TOUT(L)
  270 WRITE(NOUT,2201) (CP(L,I),I=1,NUM)
C
      WRITE(NOUT,280)
  280 FORMAT(///10X,'MASS OF PESTICIDE ON THE MASS OF SOLIDS  (MICROGRAM
     1 PER KILOGRAM)'///26X,'COMPARTMENT NUMBER'//)
      WRITE(NOUT,205) (I,I=1,NUM)
      DO 290 L=1,IOUT
      WRITE(NOUT,220) TOUT(L)
  290 WRITE(NOUT,300) (CM(L,I),I=1,NUM)
  300 FORMAT(5(9X,F7.2))
C
      RETURN
      END
C
      SUBROUTINE DIFFEQ
C
      COMMON /GEN/ NUM,H,OUTDEL,TIM,TFIN,NERR,NOUT,INTER
      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30)
     1,IPOS(30,30),ED(30,30),EP(30,30),SA(30,30),AL(30,30)
     2,DISD(30,30),DISP(30,30)
      COMMON /SOLIDS/ AM(30),AMIN(30),DAM(30),AKS(30)
      COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
      COMMON /FLUX/ R1(30),R2(30),R3(30),R4(30),R5(30),EXT(30),FNET(30)
      DIMENSION CD(30),CP(30)
C
      DO 100 I=1,NUM
C
C*****INITIALIZE NET FLUXES
C
```

EPA-287 (Cin.)
(4-76)

```
      R1(I)=0.0
      R2(I)=0.0
      R3(I)=0.0
      R4(I)=0.0
      R5(I)=0.0
C
C*****COMPUTE DISSOLVED AND PARTICULATE CONCENTRATIONS
C
      CD(I)=AF1(I)*C(I)
      CP(I)=AF2(I)*C(I)
C
C*****MASS FLUX DUE TO INFLOWS FROM OTHER COMPARTMENTS
C
      DO 110 J=1,NUM
  110 R1(I)=R1(I)+Q(J,I)*C(J)
C
C*****MASS FLUX DUE TO OUTFLOWS TO OTHER COMPARTMENTS
C
      DO 120 J=1,NUM
  120 R2(I)=R2(I)+Q(I,J)*C(I)
C
C******CHANGE IN CONCENTRATION DUE TO REACTION
C
      DO 130 K=1,9
  130 R3(I)=R3(I)+F(I,K)*C(I)*V(I)
C
C*****MASS FLUX DUE TO DISPERSION
C
      DO 140 J=1,NUM
      CD1=AF1(J)*C(J)
      CP1=C(J)-CD1
  140 R4(I)=R4(I)+DISD(I,J)*(CD1-CD(I))+DISP(I,J)*(CP1-CP(I))
C
C*****MASS FLUX DUE TO SETTLING FROM ABOVE
C
      DO 150 J=1,NUM
  150 R5(I)=R5(I)+F(J,6)*C(J)*IPOS(J,I)*V(J)
C
C*****SET UP DIFFERENTIAL EQUATION FOR EACH COMPARTMENT
C
      EXT(I)=QIN(I)*CIN(I) - QOUT(I)*C(I)
      FNET(I)=EXT(I) + R1(I) - R2(I) - R3(I) + R4(I) + R5(I)
      DC(I)=FNET(I)/V(I)
C
  100 CONTINUE
      RETURN
      END
C
```

```
      SUBROUTINE INPUTS
C
      COMMON /GEN/ NUM,H,OUTDEL,TIM,TFIN,NERR,NOUT,INTER
      COMMON /CONC/ C(30),CIN(30),DC(30),AF1(30),AF2(30),F(30,10)
      COMMON /FLOWS/ V(30),QIN(30),QOUT(30),Q(30,30)
     1,IPOS(30,30),ED(30,30),EP(30,30),SA(30,30),AL(30,30)
     2,DISD(30,30),DISP(30,30)
C
      IF(TIM.GT.1799) OUTDEL=50.
      IF(TIM.GE.2399) OUTDEL=600.
      IF(TIM.GE.1800.0) GO TO 111
      CIN(1)=0.15*EXP(-0.00045*TIM)
      IF(TIM.NE.0.0) RETURN
      WRITE(NOUT,100)
  100 FORMAT(/10X,'INPUT: CIN(1)=0.15*EXP(-0.00045*TIM)'//)
      RETURN
C
  111 CONTINUE
      CIN(1)=0.0
      IF(TIM.NE.1800.0) RETURN
      WRITE(NOUT,200) TIM,CIN(1)
  200 FORMAT(/5X,'AT TIME',F7.1,' CIN(1) SET TO ',F5.1/)
      DO 300 I=1,NUM
      DO 400 J=1,NUM
  400 Q(I,J)=Q(I,J)/3.0
      QIN(I)=QIN(I)/3.0
      QOUT(I)=QOUT(I)/3.0
  300 CONTINUE
C
      RETURN
      END
BOTTOM
Q
OK,
      ED TWOCOMP
EDIT
P999
.NULL.
C
C*****TWO COMPARTMENT MODEL FOR MASS BALANCE
C*****CORALVILLE LAKE
C*****CONSTANT COMPARTMENT VOLUMES
C*****PROGRAMMER: RAO       APRIL 1981
C
      COMMON TIM,Q,AMIN,AKS,V1,V2,E,A,AL,AM(2),DAM(2)
      DIMENSION AML(2)
      DIMENSION A1(2),A2(2),A3(2),A4(2)
      NUM=2
      TIM=0.0
      H=1
      AMIN=0.00024
      AM(1)=0.00005
      AM(2)=0.3
      OUTDEL=600
      TSAV=OUTDEL
      Q=3.3519
      V1=46.2484
      V2=5.952
      A=19.836
      AL=1.317
      WRITE(1,555)
  555 FORMAT(/'ENTER ENDING TIME FOR SIMULATION (DAYS)')
      READ(1,*) TFIN
      WRITE(1,888)
  888 FORMAT(/'ENTER INFLOW SOLIDS CONC (KG/L)')
      READ(1,*) AMIN
      WRITE(1,999)
  999 FORMAT(/'ENTER KS (1/DAY)')
      READ(1,*) AKS
      WRITE(1,998)
  998 FORMAT(/'ENTER E (M**2/DAY)')
      READ(1,*) E
      DTHLF=0.5*H
      WRITE(1,332)
  332 FORMAT(/'TIME',5X,'M IN WATER',3X,'M IN SEDIMENT',5X,'FLUX',10X,
     1'FLUX',8X,'NET FLUX',/'DAYS',8X,'KG/L',10X,'KG/L',6X,
     2'TO SEDIMENT',3X,'FROM SEDIMENT',2X,'TO SEDIMENT',
     3,/39X,'KG/DAY',8X,'KG/DAY',8X,'KG/DAY')
      FLUX1=AKS*AM(1)*V1*1.E09
      FLUX2=(E*A*(AM(2)-AM(1)))/AL
      FLUX2=FLUX2*1.E09
```

Table 3. TWOCOMP code for Solids balance in a 2 - compartment reservoir with constant volume sediment compartment

```
      FLUX=FLUX1-FLUX2
      WRITE(1,333) TIM,AM,FLUX1,FLUX2,FLUX
C
   50 CONTINUE
C
      DO 200 I=1,2
  200 AML(I)=AM(I)
      CALL DIFFEM
      DO 100 I=1,NUM
  100 AML(I)=AM(I)
C
      CALL DIFFEM
      DO 110 I=1,NUM
      A1(I)=DAM(I)
  110 AM(I)=AML(I)+DTHLF*A1(I)
      CALL DIFFEM
      DO 120 I=1,NUM
      A2(I)=DAM(I)
  120 AM(I)=AML(I)+DTHLF*A2(I)
      CALL DIFFEM
      DO 130 I=1,NUM
      A3(I)=DAM(I)
  130 AM(I)=AML(I)+H*A3(I)
      CALL DIFFEM
      DO 140 I=1,NUM
      A4(I)=DAM(I)
  140 AM(I)=AML(I)+H*(A1(I)+2.*A2(I)+2.*A3(I)+A4(I))/6.
      TIM=TIM+H
      TNEX=AMINO(TSAV,TFIN)
      IF(TIM.GE.TNEX) GO TO 150
      GO TO 50
  150 CONTINUE
      FLUX1=AKS*AM(1)*V1*1.E09
      FLUX2=(E*A*(AM(2)-AM(1)))/AL
      FLUX2=FLUX2*1.E09
      FLUX=FLUX1-FLUX2
      WRITE(1,333) TIM,AM,FLUX1,FLUX2,FLUX
  333 FORMAT(/F5.0,2X,5(E12.4,2X))
C
      TSAV=TSAV+OUTDEL
      IF(TIM.GE.TFIN) GO TO 444
      GO TO 50
  444 CALL EXIT
      END
      SUBROUTINE DIFFEM
      COMMON TIM,Q,AMIN,AKS,V1,V2,E,A,AL,AM(2),DAM(2)
      DAM(1)=Q*(AMIN-AM(1)) - AKS*V1*AM(1) + E*A*(AM(2)-AM(1))/AL
      DAM(1)=DAM(1)/V1
      DAM(2)=AKS*V1*AM(1)/V2 + E*A*(AM(1)-AM(2))/(AL*V2)
      RETURN
      END
BOTTOM
```

```
      ED TWOCOMP1
EDIT
P999
.NULL.
C
C*****TWO COMPARTMENT MODEL FOR MASS BALANCE
C*****CORALVILLE LAKE
C*****VARIABLE COMPARTMENT VOLUMES
C*****PROGRAMMER: RAO       APRIL 1981
C
      COMMON TIM,Q,AMIN,AKS,V1,V2,E,A,AL,AM(2),DAM(2)
      DIMENSION AML(2)
      DIMENSION A1(2),A2(2),A3(2),A4(2)
      NUM=2
      TIM=0.0
      H=1
      AMIN=0.00024
      AM(1)=0.00005
      AM(2)=0.3
      OUTDEL=600
      TSAV=OUTDEL
      Q=3.3519
      VOL1=46.2484
      VOL2=5.952
      A=19.836
      AL=1.317
      WRITE(1,555)
  555 FORMAT(/'ENTER ENDING TIME FOR SIMULATION (DAYS)')
      READ(1,*) TFIN
      WRITE(1,888)
  888 FORMAT(/'ENTER INFLOW SOLIDS CONC (KG/L)')
      READ(1,*) AMIN
      WRITE(1,999)
  999 FORMAT(/'ENTER KS (1/DAY)')
      READ(1,*) AKS
      WRITE(1,998)
```

Table 4. TWOCOMP1 code for solids balance in a 2 - compartment reservoir with variable volume in the sediment compartment

```
  998 FORMAT(/'ENTER E (M**2/DAY)')
      READ(1,*) E
      WRITE(1,996)
  996 FORMAT(/'ENTER VOLUME INCREASE FACTOR')
      READ(1,*) FAC
      DTHLF=0.5*H
      WRITE(1,332)
  332 FORMAT(/'TIME',5X,'M IN WATER',3X,'M IN SEDIMENT',5X,'FLUX',10X,
     1'FLUX',8X,'NET FLUX',/'DAYS',8X,'KG/L',10X,'KG/L',6X,
     2'TO SEDIMENT',3X,'FROM SEDIMENT',2X,'TO SEDIMENT',
     3,/39X,'KG/DAY',8X,'KG/DAY',8X,'KG/DAY')
      V1=VOL1
      V2=VOL2
      FLUX1=AKS*AM(1)*V1*1.E09
      FLUX2=(E*A*(AM(2)-AM(1)))/AL
      FLUX2=FLUX2*1.E09
      FLUX=FLUX1-FLUX2
      WRITE(1,333) TIM,AM,FLUX1,FLUX2,FLUX
      WRITE(1,995) V1,V2
C
   50 CONTINUE
      V1=VOL1-5.952*(FAC-1)*TIM/TFIN
      V2=VOL2+5.952*(FAC-1)*TIM/TFIN
C
      DO 200 I=1,2
  200 AML(I)=AM(I)
      CALL DIFFEM
      DO 100 I=1,NUM
  100 AML(I)=AM(I)
C
      CALL DIFFEM
      DO 110 I=1,NUM
      A1(I)=DAM(I)
  110 AM(I)=AML(I)+DTHLF*A1(I)
      CALL DIFFEM
      DO 120 I=1,NUM
      A2(I)=DAM(I)
  120 AM(I)=AML(I)+DTHLF*A2(I)
      CALL DIFFEM
      DO 130 I=1,NUM
      A3(I)=DAM(I)
  130 AM(I)=AML(I)+H*A3(I)
      CALL DIFFEM
      DO 140 I=1,NUM
      A4(I)=DAM(I)
  140 AM(I)=AML(I)+H*(A1(I)+2.*A2(I)+2.*A3(I)+A4(I))/6.
      TIM=TIM+H
      TNEX=AMINO(TSAV,TFIN)
      IF(TIM.GE.TNEX) GO TO 150
      GO TO 50
  150 CONTINUE
      FLUX1=AKS*AM(1)*V1*1.E09
      FLUX2=(E*A*(AM(2)-AM(1)))/AL
      FLUX2=FLUX2*1.E09
      FLUX=FLUX1-FLUX2
      WRITE(1,333) TIM,AM,FLUX1,FLUX2,FLUX
  333 FORMAT(/F5.0,2X,5(E12.4,2X))
C
      WRITE(1,995) V1,V2
  995 FORMAT(/15X,'( V1=',F7.3,' M CU. M',5X,'V2=',F7.3,' M CU. M )')
C
      TSAV=TSAV+OUTDEL
      IF(TIM.GE.TFIN) GO TO 444
      GO TO 50
  444 CALL EXIT
      END
      SUBROUTINE DIFFEM
      COMMON TIM,Q,AMIN,AKS,V1,V2,E,A,AL,AM(2),DAM(2)
      DAM(1)=Q*(AMIN-AM(1)) - AKS*V1*AM(1) + E*A*(AM(2)-AM(1))/AL
      DAM(1)=DAM(1)/V1
      DAM(2)=AKS*V1*AM(1)/V2 + E*A*(AM(1)-AM(2))/(AL*V2)
      RETURN
      END
BOTTOM
```

SAMPLE INPUT FOR TOXIC

```
OK, ED DATA
EDIT
P999
.NULL.
DIELDRIN
9,1.0,600.0,3600 / NUM,H,OUTDEL,TFIN
6.612,6.612,6.612,2.015,13.224,13.224,1.0,2.015,2.015
3.3519,/ INFLOWS FROM OUTSIDE THE SYSTEM
0,0,0,0,0,3.3519,/ OUTFLOWS TO OUTSIDE THE SYSTEM
0,3.3519,/FLOWS OUT OF COMPARTMENT 1
0,0,1.67595,0,1.67595,/ FLOWS OUT OF COMPARTMENT 2
0,0,0,0,0,1.67595,/ FLOWS OUT OF COMPARTMENT 3
0,/ FLOWS OUT OF COMPARTMENT 4
0,0,0,0,0,1.67595,/ FLOWS OUT OF COMPARTMENT 5
0,/ FLOWS OUT OF COMPARTMENT 6
0,/ FLOWS OUT OF COMPARTMENT 7
0,/ FLOWS OUT OF COMPARTMENT 8
0,/ FLOWS OUT OF COMPARTMENT 9
0.025,0.025,0.025,2.25,0.025,0.025,0.0,2.25,2.25 /  INITIAL CONCENTRATIONS
0.000226,0.000126,0.000049,0.36,0.000150,0.000096,0.00005,0.577,0.424
6700,6700,6700,6700,6700,6700,6700,6700,6700 / PARTITION COEFFICIENTS, PC
0.0,1.0,0.0,0.00015,/ DISPERSION COEFFICIENTS
1.0,0.0,1.0,.001,/
0.0,1.0,0,0,0,.001,/
.00015,/
0.0,.001,0,0,0,1.0,0,.00015,0
0,0,.001,0,1.0,0,0,0,.00015
0,/
0,0,0,0,.00015,/
0,0,0,0,0,.00015,/
0,.00057,0,6.612,/ INTERFACE SURFACE AREAS, MILLION SQ. M
.00057,0,.00057,0,6.612,/
0,.00057,0,0,0,6.612,/
6.612,/
0,6.612,0,0,0,.00136,0,6.612,0
0,0,6.612,0,.00136,0,0,0,6.612
0,/
0,0,0,0,6.612,/
0,0,0,0,0,6.612,/
1,11641,,.65,/ DISTANCES BETWEEN COMPARTMENTS, M
```

Table 5. DATA file for input to TOXIC

```
11641,1,11641,1,1.5,/
1,568,1,1,1,1.5,/
.65,/
1,1.5,1,1,1,1,1,1.15,1
1,1,1.5,1,11641,1,1,1,1.15
1,/
1,1,1,1,1.15,/
1,1,1,1,1,1.15,/
1,1,1,.305,2,2,1,.305,.305
/ AQY :  PHOTOSYNTHESIS
/ AKI :  QUANTUM YIELD
/ OXK :  OXIDATION,DISSOLVED PHASE
/ RO2
/ BXB :  BASE CATALYSED HYDROLYSIS
/ AKA :  ACID CATALYSED HYDROLYSIS
/ AKN :  NEUTRAL CATALYSED HYDROLYSIS
/ PH
.000325,.000325,.000325,.000325,.000325,.000325,0,.000325,.000325
/ GRM
/ YLD
/ HKS
/ XMB
.4,.4,.4,0,.4,.4,/ AKS :  SETTLING RATE CONSTANT
0,0,0,1,/ 1 IS ABOVE 4
0,0,0,0,1,/ 2 IS ABOVE 5
0,0,0,0,0,1,/ 3 IS ABOVE 6
/
0,0,0,0,0,0,0,1,0
0,0,0,0,0,0,0,0,1
/
/
/
0,0,0,.0052,,,,.0052,.0052
1,1,1,1,1,1,1,1,1
/ BKBP
/ AKAP
/ AKNP
/ PHP
/ GRMP
/ YLDP
/ HKSP
/ XMBP
BOTTOM
```

SAMPLE OUTPUTS

TWOCOMP
TWOCOMP1
PESTY2 - 2 compartment
TOXIC - 9 compartment
TOXIC - 25 compartment

```
OK, r *twocomp

ENTER ENDING TIME FOR SIMULATION (DAYS)
3600

ENTER INFLOW SOLIDS CONC (KG/L)
.00014

ENTER KS (1/DAY)
.4

ENTER E (M**2/DAY)
.0001
                                               FLUX               FLUX            NET FLUX
TIME      M IN WATER      M IN SEDIMENT     TO SEDIMENT      FROM SEDIMENT      TO SEDIMENT
DAYS        KG/L              KG/L             KG/DAY            KG/DAY            KG/DAY

   0.     0.5000E-04       0.3000E 00       0.9250E 06       0.4518E 06       0.4732E 06
 600.     0.4440E-04       0.3327E 00       0.8213E 06       0.5010E 06       0.3203E 06
1200.     0.4660E-04       0.3646E 00       0.8620E 06       0.5491E 06       0.3129E 06
1800.     0.4874E-04       0.3958E 00       0.9017E 06       0.5960E 06       0.3057E 06
2400.     0.5084E-04       0.4262E 00       0.9405E 06       0.6418E 06       0.2987E 06
3000.     0.5289E-04       0.4559E 00       0.9785E 06       0.6866E 06       0.2918E 06
3600.     0.5489E-04       0.4850E 00       0.1016E 07       0.7304E 06       0.2851E 06
```

Table 6. TWOCOMP output for hypothetical solids balance in Coralville Reservoir

```
OK, r *twocomp1

ENTER ENDING TIME FOR SIMULATION (DAYS)
3600

ENTER INFLOW SOLIDS CONC (KG/L)
.00014

ENTER KS (1/DAY)
.4

ENTER E (M**2/DAY)
.0001

ENTER VOLUME INCREASE FACTOR
1.5

TIME      M IN WATER   M IN SEDIMENT      FLUX            FLUX           NET FLUX
DAYS         KG/L           KG/L       TO SEDIMENT   FROM SEDIMENT    TO SEDIMENT
                                          KG/DAY          KG/DAY          KG/DAY

   0.     0.5000E-04    0.3000E 00    0.9250E 06     0.4518E 06      0.4732E 06
                ( V1= 46.248 M CU. M      V2=   5.952 M CU. M )
 600.     0.4471E-04    0.3314E 00    0.8182E 06     0.4990E 06      0.3192E 06
                ( V1= 45.753 M CU. M      V2=   6.447 M CU. M )
1200.     0.4711E-04    0.3596E 00    0.8527E 06     0.5415E 06      0.3112E 06
                ( V1= 45.257 M CU. M      V2=   6.943 M CU. M )
1800.     0.4936E-04    0.3852E 00    0.8838E 06     0.5802E 06      0.3037E 06
                ( V1= 44.761 M CU. M      V2=   7.439 M CU. M )
2400.     0.5150E-04    0.4087E 00    0.9119E 06     0.6154E 06      0.2965E 06
                ( V1= 44.265 M CU. M      V2=   7.935 M CU. M )
3000.     0.5354E-04    0.4301E 00    0.9374E 06     0.6478E 06      0.2897E 06
                ( V1= 43.769 M CU. M      V2=   8.431 M CU. M )
3600.     0.5550E-04    0.4499E 00    0.9607E 06     0.6776E 06      0.2831E 06
                ( V1= 43.273 M CU. M      V2=   8.927 M CU. M )
```

Table 7. TWOCOMP1 output for hypothetical solids balance in Coralville Reservoir (variable volume sediment compartment)

```
OK, o twodat 1 1
OK, seg #toxic


 INPUT DATA FOR        IN
 NUMBER OF COMPARTMENTS=     2
 STEP SIZE FOR CALCULATIONS=        1.00 DAYS
 TIME BETWEEN OUTPUT POINTS=      600.00 DAYS
 TIME FOR SIMULATION        =    3600.00 DAYS

COMPARTMENT     VOLUME,MILLION CU.M     INFLOW, MILLION CU.M     OUTFLOW, MILLION CU.M
    1                46.2840                  3.3519                  3.3519
    2                 5.9520                  0.0000                  0.0000
                   INTERFLOW MATRIX FOR COMPARTMENTS
  0.0000  0.0000
  0.0000  0.
QUIT.
OK, c;lose
QUIT.
OK, close all
OK, o twodat 1 1
OK, seg #pest1

DO YOU WANT INTERMEDIATE OUTPUT (1=YES),(2=NO) ?
2


 INPUT DATA FOR DIELDRIN
 NUMBER OF COMPARTMENTS=     2
 STEP SIZE FOR CALCULATIONS=        1.00 DAYS
 TIME BETWEEN OUTPUT POINTS=      600.00 DAYS
 TIME FOR SIMULATION        =    3600.00 DAYS

COMPARTMENT     VOLUME,MILLION CU.M     INFLOW, MILLION CU.M     OUTFLOW, MILLION CU.M
    1                46.2840                  3.3519                  3.3519
    2                 5.9520                  0.0000                  0.0000
                   INTERFLOW MATRIX FOR COMPARTMENTS
  0.0000  0.0000
  0.0000  0.0000
```

Table 8. Sample output for PESTY2 or two - compartment TOXIC

```
COMPARTMENT     INITIAL            MASS OF            PARTITION        FRACTION IN
             CONCENTRATION    SUSPENDED SOLIDS     COEFFICIENT     DISSOLVED PHASE
     1           0.0250          0.600E-03            1000.             0.625
     2           2.2500          0.321E 01            1000.             0.000
                            DISPERSION COEFFICIENTS

 0.0E 00 0.1E-03 0.1E-03 0.0E 00
                               INTERFACE AREAS

  0.000  19.836  19.836   0.000
                         MEAN LENGTH BETWEEN COMPARTMENTS

 0.100E 010.132E 010.132E 010.100E 01
                          SETTLING RATE CONSTANTS

   0.40   0.00

                         COMPARTMENT POSITION MATRIX
                   0   1   0   0

               PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)
                         IN THE DISSOLVED PHASE

  CMPN  PHOTOLYSIS   OXIDATION   HYDROLYSIS    BIOLYSIS  VOLATILIZATION
   1    0.0000000    0.0000000   0.0000000    0.0000000   0.0003250
   2    0.0000000    0.0000000   0.0000000    0.0000000   0.0003250

               PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)
                        IN THE PARTICULATE PHASE

                 CMPN  OXIDATION   HYDROLYSIS   BIOLYSIS
                  1    0.0000000   0.0000000    0.0000000
                  2    0.0052000   0.0000000    0.0000000

                    SIMULATION HALTED AT TIME =  3600.0
```

Table 8. (continued)

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-78)

```
          TOTAL CONCENTRATION OF PESTICIDE OVER TIME (PPB)
TIME(DAYS)                 COMPARTMENT NUMBER

              1       2
     0.0  0.0250  2.2500
   600.0  0.0131  2.9135
  1200.0  0.0100  2.2720
  1800.0  0.0076  1.7364
  2400.0  0.0058  1.3256
  3000.0  0.0044  1.0119
  3600.0  0.0034  0.7725

          DISSOLVED CONCENTRATION OF PESTICIDE OVER TIME     (PPB)
TIME(DAYS)                 COMPARTMENT NUMBER

              1       2
     0.0  0.0156  0.0007
   600.0  0.0082  0.0009
  1200.0  0.0062  0.0007
  1800.0  0.0048  0.0005
  2400.0  0.0036  0.0004
  3000.0  0.0028  0.0003
  3600.0  0.0021  0.0002

          PARTICULATE CONCENTRATION OF PESTICIDE OVER TIME   (PPB)
TIME(DAYS)                 COMPARTMENT NUMBER

              1       2
     0.0  0.0094  2.2493
   600.0  0.0049  2.9126
  1200.0  0.0037  2.2713
  1800.0  0.0029  1.7358
  2400.0  0.0022  1.3252
  3000.0  0.0017  1.0116
  3600.0  0.0013  0.7722

          MASS OF PESTICIDE ON THE MASS OF SOLIDS  (MICROGRAM PER KILOGRAM)

TIME(DAYS)                 COMPARTMENT NUMBER

              1         2
    0.0    15.63      0.70
  600.0     8.18      0.91
 1200.0     6.25      0.71
 1800.0     4.77      0.54
 2400.0     3.64      0.41
 3000.0     2.78      0.32
 3600.0     2.12      0.24
```

Tabel 8. (con't)

```
INPUT DATA FOR          IN
NUMBER OF COMPARTMENTS=        9
STEP SIZE FOR CALCULATIONS=        1.00 DAYS
TIME BETWEEN OUTPUT POINTS=     600.00 DAYS
TIME FOR SIMULATION        =   7200.00 DAYS

COMPARTMENT      VOLUME,MILLION CU.M      INFLOW, MILLION CU.M      OUTFLOW, MILLION CU.M
     1                     6.6120                  3.3519                  0.0000
     2                     6.6120                  0.0000                  0.0000
     3                     6.6120                  0.0000                  0.0000
     4                     2.0150                  0.0000                  0.0000
     5                    13.2240                  0.0000                  0.0000
     6                    13.2240                  0.0000                  3.3519
     7                     1.0000                  0.0000                  0.0000
     8                     2.0150                  0.0000                  0.0000
     9                     2.0150                  0.0000                  0.0000
                          INTERFLOW MATRIX FOR COMPARTMENTS
  0.0000   3.3519   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   1.6759   0.0000   1.6759   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   1.6759   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   1.6759   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
COMPARTMENT       INITIAL             MASS OF            PARTITION         FRACTION IN
               CONCENTRATION     SUSPENDED SOLIDS       COEFFICIENT      DISSOLVED PHASE
     1            0.0250            0.226E-03              6700.             0.398
     2            0.0250            0.126E-03              6700.             0.542
     3            0.0250            0.490E-04              6700.             0.753
     4            2.2500            0.360E 00              6700.             0.000
     5            0.0250            0.150E-03              6700.             0.499
     6            0.0250            0.960E-04              6700.             0.609
     7            0.0000            0.500E-04              6700.             0.749
     8            2.2500            0.577E 00              6700.             0.000
     9            2.2500            0.424E 00              6700.             0.000
```

Table 9. Sample Output for the 9 - compartment TOXIC model

```
                    DISPERSION COEFFICIENTS
0.0E 00 0.1E 01 0.0E 00 0.1E-03 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00
0.1E 01 0.0E 00 0.1E 01 0.1E-02 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00
0.0E 00 0.1E 01 0.0E 00 0.0E 00 0.0E 00 0.1E-02 0.0E 00 0.0E 00 0.0E 00
0.1E-03 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00
0.0E 00 0.1E-02 0.0E 00 0.0E 00 0.0E 00 0.1E 01 0.0E 00 0.1E-03 0.0E 00
0.0E 00 0.0E 00 0.1E-02 0.0E 00 0.1E 01 0.0E 00 0.0E 00 0.0E 00 0.1E-03
0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00
0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.1E-03 0.0E 00 0.0E 00 0.0E 00 0.0E 00
0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.0E 00 0.1E-03 0.0E 00 0.0E 00 0.0E 00
                      INTERFACE AREAS
   0.000    0.001    0.000    6.612    0.000    0.000    0.000    0.000    0.000
   0.001    0.000    0.001    0.000    6.612    0.000    0.000    0.000    0.000
   0.000    0.001    0.000    0.000    0.000    6.612    0.000    0.000    0.000
   6.612    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
   0.000    6.612    0.000    0.000    0.000    0.001    0.000    6.612    0.000
   0.000    0.000    6.612    0.000    0.001    0.000    0.000    0.000    6.612
   0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000
   0.000    0.000    0.000    0.000    6.612    0.000    0.000    0.000    0.000
   0.000    0.000    0.000    0.000    0.000    6.612    0.000    0.000    0.000
                 MEAN LENGTH BETWEEN COMPARTMENTS
 0.100E 010.116E 050.100E 010.650E 000.100E 010.100E 010.100E 010.100E 010.100E 01
 0.116E 050.100E 010.116E 050.100E 010.150E 010.100E 010.100E 010.100E 010.100E 01
 0.100E 010.568E 030.100E 010.100E 010.100E 010.150E 010.100E 010.100E 010.100E 01
 0.650E 000.100E 010.100E 010.100E 010.100E 010.100E 010.100E 010.100E 010.100E 01
 0.100E 010.150E 010.100E 010.100E 010.100E 010.100E 010.100E 010.115E 010.100E 01
```

```
0.100E 010.100E 010.150E 010.100E 010.116E 050.100E 010.100E 010.100E 010.115E 01
0.100E 010.100E 010.100E 010.100E 010.100E 010.100E 010.100E 010.100E 010.100E 01
0.100E 010.100E 010.100E 010.100E 010.115E 010.100E 010.100E 010.100E 010.100E 01
0.100E 010.100E 010.100E 010.100E 010.100E 010.115E 010.100E 010.100E 010.100E 01
                    SETTLING RATE CONSTANTS

  0.60   0.60   0.60   0.00   0.60   0.60   0.00   0.00   0.00

                    COMPARTMENT POSITION MATRIX
                 0    0    0    1    0    0    0    0    0
                 0    0    0    0    1    0    0    0    0
                 0    0    0    0    0    1    0    0    0
                 0    0    0    0    0    0    0    0    0
                 0    0    0    0    0    0    0    1    0
                 0    0    0    0    0    0    0    0    1
                 0    0    0    0    0    0    0    0    0
                 0    0    0    0    0    0    0    0    0
                 0    0    0    0    0    0    0    0    0

           PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)
                     IN THE DISSOLVED PHASE

CMPN  PHOTOLYSIS   OXIDATION   HYDROLYSIS    BIOLYSIS   VOLATILIZATION
  1   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  2   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  3   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  4   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  5   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  6   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  7   0.0000000    0.0000000   0.0000000    0.0000000    0.0000000
  8   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250
  9   0.0000000    0.0000000   0.0000000    0.0000000    0.0003250

           PSEUDO-FIRST-ORDER RATE CONSTANTS (PER DAY)
                    IN THE PARTICULATE PHASE
```

```
CMPN  OXIDATION  HYDROLYSIS   BIOLYSIS
  1   0.0000000   0.0000000   0.0000000
  2   0.0000000   0.0000000   0.0000000
  3   0.0000000   0.0000000   0.0000000
  4   0.0052000   0.0000000   0.0000000
  5   0.0000000   0.0000000   0.0000000
  6   0.0000000   0.0000000   0.0000000
  7   0.0000000   0.0000000   0.0000000
  8   0.0052000   0.0000000   0.0000000
  9   0.0052000   0.0000000   0.0000000

     R1   = FLUX DUE TO INFLOW FROM OTHER COMPARTMENTS

     R2   = FLUX DUE TO OUTFLOW TO  OTHER COMPARTMENTS

     R3   = FLUX DUE TO REACTION

     R4   = FLUX DUE TO DISPERSION (NET INFLOW)

     R5   = FLUX DUE TO SETTLING FROM ABOVE

     EXT  = FLUX DUE FLOWS TO OR FROM OUTSIDE THE SYSTEM

     FNET= NET FLUX TO EACH COMPARTMENT

     ALL UNITS IN KG/DAY


                     TIME=   600.0
CMPN      R1               R2               R3               R4               R5
  1   0.000000E 00     0.791232E-01     0.564203E-01     0.751043E-02     0.000000E 00
  2   0.791232E-01     0.513415E-01     0.278341E-01     0.128968E-09     0.000000E 00
  3   0.256707E-01     0.161941E-01     0.949010E-02     -.123785E-04     0.000000E 00
  4   0.000000E 00     0.000000E 00     0.518014E-01     -.751043E-02     0.564001E-01
  5   0.256707E-01     0.168175E-01     0.399301E-01     0.320812E-02     0.278162E-01
  6   0.330116E-01     0.000000E 00     0.213023E-01     0.174716E-02     0.947447E-02
  7   0.000000E 00     0.000000E 00     0.000000E 00     0.000000E 00     0.000000E 00
  8   0.000000E 00     0.000000E 00     0.388419E-01     -.318916E-02     0.399086E-01
  9   0.000000E 00     0.000000E 00     0.211412E-01     -.173478E-02     0.212844E-01
```

```
                                        TIME=  1200.0
CMPN     R1             R2             R3             R4             R5
  1   0.000000E 00   0.604994E-01   0.431403E-01   0.590076E-02   0.000000E 00
  2   0.604994E-01   0.392573E-01   0.212828E-01   0.986114E-10   0.000000E 00
  3   0.196286E-01   0.123828E-01   0.725659E-02   -.943812E-05   0.000000E 00
  4   0.000000E 00   0.000000E 00   0.406939E-01   -.590076E-02   0.431248E-01
  5   0.196286E-01   0.128829E-01   0.305880E-01   0.253113E-02   0.212692E-01
  6   0.252657E-01   0.000000E 00   0.163079E-01   0.135132E-02   0.724464E-02
  7   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00
  8   0.000000E 00   0.000000E 00   0.306493E-01   -.251670E-02   0.305715E-01
  9   0.000000E 00   0.000000E 00   0.163524E-01   -.134187E-02   0.162942E-01

                                        TIME=  1800.0
CMPN     R1             R2             R3             R4             R5
  1   0.000000E 00   0.461874E-01   0.329348E-01   0.451022E-02   0.000000E 00
  2   0.461874E-01   0.299704E-01   0.162480E-01   0.752837E-10   0.000000E 00
  3   0.149852E-01   0.945349E-02   0.553995E-02   -.720397E-05   0.000000E 00
  4   0.000000E 00   0.000000E 00   0.311040E-01   -.451022E-02   0.329230E-01
  5   0.149852E-01   0.983635E-02   0.233546E-01   0.193603E-02   0.162376E-01
  6   0.192898E-01   0.000000E 00   0.124510E-01   0.103261E-02   0.553082E-02
  7   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00
  8   0.000000E 00   0.000000E 00   0.234435E-01   -.192502E-02   0.233420E-01
  9   0.000000E 00   0.000000E 00   0.124958E-01   -.102540E-02   0.124406E-01

                                        TIME=  2400.0
CMPN     R1             R2             R3             R4             R5
  1   0.000000E 00   0.352586E-01   0.251418E-01   0.344319E-02   0.000000E 00
  2   0.352586E-01   0.228788E-01   0.124035E-01   0.574701E-10   0.000000E 00
  3   0.114394E-01   0.721662E-02   0.422909E-02   -.549930E-05   0.000000E 00
  4   0.000000E 00   0.000000E 00   0.237454E-01   -.344319E-02   0.251328E-01
  5   0.114394E-01   0.750894E-02   0.178286E-01   0.147810E-02   0.123955E-01
  6   0.147256E-01   0.000000E 00   0.950495E-02   0.788332E-03   0.422213E-02
  7   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00   0.000000E 00
  8   0.000000E 00   0.000000E 00   0.178985E-01   -.146970E-02   0.178190E-01
  9   0.000000E 00   0.000000E 00   0.953975E-02   -.782830E-03   0.949696E-02
```

```
                                   TIME=  3000.0

CMPN       R1                R2                R3                R4                R5
  1    0.000000E 00      0.269157E-01      0.191927E-01      0.262848E-02      0.000000E 00
  2    0.269157E-01      0.174652E-01      0.946855E-02      0.438715E-10      0.000000E 00
  3    0.873262E-02      0.550902E-02      0.322840E-02      -.419805E-05      0.000000E 00
  4    0.000000E 00      0.000000E 00      0.181269E-01      -.262848E-02      0.191859E-01
  5    0.873262E-02      0.573217E-02      0.136100E-01      0.112836E-02      0.946248E-02
  6    0.112412E-01      0.000000E 00      0.725589E-02      0.601799E-03      0.322309E-02
  7    0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00
  8    0.000000E 00      0.000000E 00      0.136634E-01      -.112194E-02      0.136027E-01
  9    0.000000E 00      0.000000E 00      0.728248E-02      -.597599E-03      0.724979E-02

                                   TIME=  3600.0

CMPN       R1                R2                R3                R4                R5
  1    0.000000E 00      0.205469E-01      0.146513E-01      0.200652E-02      0.000000E 00
  2    0.205469E-01      0.133326E-01      0.722810E-02      0.334907E-10      0.000000E 00
  3    0.666630E-02      0.420547E-02      0.246450E-02      -.320471E-05      0.000000E 00
  4    0.000000E 00      0.000000E 00      0.138377E-01      -.200652E-02      0.146461E-01
  5    0.666630E-02      0.437582E-02      0.103896E-01      0.861363E-03      0.722346E-02
  6    0.858130E-02      0.000000E 00      0.553900E-02      0.459398E-03      0.246044E-02
  7    0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00
  8    0.000000E 00      0.000000E 00      0.104303E-01      -.856466E-03      0.103840E-01
  9    0.000000E 00      0.000000E 00      0.555926E-02      -.456192E-03      0.553434E-02

                                   TIME=  4200.0

CMPN       R1                R2                R3                R4                R5
  1    0.000000E 00      0.156851E-01      0.111845E-01      0.153173E-02      0.000000E 00
  2    0.156851E-01      0.101778E-01      0.551778E-02      0.255660E-10      0.000000E 00
  3    0.508892E-02      0.321037E-02      0.188135E-02      -.244641E-05      0.000000E 00
  4    0.000000E 00      0.000000E 00      0.105633E-01      -.153173E-02      0.111805E-01
  5    0.508892E-02      0.334041E-02      0.793120E-02      0.657551E-03      0.551424E-02
  6    0.655078E-02      0.000000E 00      0.422836E-02      0.350698E-03      0.187825E-02
  7    0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00      0.000000E 00
  8    0.000000E 00      0.000000E 00      0.796234E-02      -.653813E-03      0.792693E-02
  9    0.000000E 00      0.000000E 00      0.424386E-02      -.348250E-03      0.422480E-02
```

```
                          TIME=   4800.0

CMPN     R1              R2              R3              R4              R5
  1   0.000000E 00    0.119737E-01    0.853805E-02    0.116930E-02    0.000000E 00
  2   0.119737E-01    0.776955E-02    0.421216E-02    0.195166E-10    0.000000E 00
  3   0.388478E-02    0.245073E-02    0.143618E-02    -.186754E-05    0.000000E 00
  4   0.000000E 00    0.000000E 00    0.806388E-02    -.116930E-02    0.853499E-02
  5   0.388478E-02    0.255000E-02    0.605451E-02    0.501957E-03    0.420946E-02
  6   0.500073E-02    0.000000E 00    0.322784E-02    0.267715E-03    0.143382E-02
  7   0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00
  8   0.000000E 00    0.000000E 00    0.607824E-02    -.499104E-03    0.605125E-02
  9   0.000000E 00    0.000000E 00    0.323967E-02    -.265846E-03    0.322512E-02

                          TIME=   5400.0

CMPN     R1              R2              R3              R4              R5
  1   0.000000E 00    0.914044E-02    0.651777E-02    0.892617E-03    0.000000E 00
  2   0.914044E-02    0.593112E-02    0.321548E-02    0.148986E-10    0.000000E 00
  3   0.296556E-02    0.187084E-02    0.109635E-02    -.142564E-05    0.000000E 00
  4   0.000000E 00    0.000000E 00    0.615579E-02    -.892618E-03    0.651544E-02
  5   0.296556E-02    0.194662E-02    0.462189E-02    0.383187E-03    0.321342E-02
  6   0.381746E-02    0.000000E 00    0.246407E-02    0.204368E-03    0.109455E-02
  7   0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00
  8   0.000000E 00    0.000000E 00    0.464003E-02    -.381008E-03    0.461940E-02
  9   0.000000E 00    0.000000E 00    0.247309E-02    -.202942E-03    0.246199E-02

                          TIME=   6000.0

CMPN     R1              R2              R3              R4              R5
  1   0.000000E 00    0.697763E-02    0.497553E-02    0.681407E-03    0.000000E 00
  2   0.697763E-02    0.452769E-02    0.245463E-02    0.113733E-10    0.000000E 00
  3   0.226385E-02    0.142816E-02    0.836932E-03    -.108830E-05    0.000000E 00
  4   0.000000E 00    0.000000E 00    0.469921E-02    -.681407E-03    0.497375E-02
  5   0.226385E-02    0.148601E-02    0.352826E-02    0.292516E-03    0.245306E-02
  6   0.291417E-02    0.000000E 00    0.188102E-02    0.156011E-03    0.835554E-03
  7   0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00
  8   0.000000E 00    0.000000E 00    0.354210E-02    -.290853E-03    0.352636E-02
  9   0.000000E 00    0.000000E 00    0.188791E-02    -.154922E-03    0.187944E-02
```

```
                             TIME=  6600.0
CMPN      R1              R2              R3              R4              R5
  1   0.000000E 00    0.532658E-02    0.379822E-02    0.520171E-03    0.000000E 00
  2   0.532658E-02    0.345635E-02    0.187381E-02    0.868212E-11    0.000000E 00
  3   0.172817E-02    0.109023E-02    0.638897E-03    -.830790E-06    0.000000E 00
  4   0.000000E 00    0.000000E 00    0.358728E-02    -.520171E-03    0.379686E-02
  5   0.172817E-02    0.113439E-02    0.269340E-02    0.223300E-03    0.187261E-02
  6   0.222462E-02    0.000000E 00    0.143593E-02    0.119095E-03    0.637844E-03
  7   0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00
  8   0.000000E 00    0.000000E 00    0.270395E-02    -.222030E-03    0.269195E-02
  9   0.000000E 00    0.000000E 00    0.144119E-02    -.118264E-03    0.143472E-02


                             TIME=  7200.0
CMPN      R1              R2              R3              R4              R5
  1   0.000000E 00    0.406620E-02    0.289948E-02    0.397086E-03    0.000000E 00
  2   0.406620E-02    0.263850E-02    0.143043E-02    0.662773E-11    0.000000E 00
  3   0.131925E-02    0.832257E-03    0.487720E-03    -.634207E-06    0.000000E 00
  4   0.000000E 00    0.000000E 00    0.273844E-02    -.397086E-03    0.289844E-02
  5   0.131925E-02    0.865969E-03    0.205609E-02    0.170464E-03    0.142951E-02
  6   0.169823E-02    0.000000E 00    0.109616E-02    0.909150E-04    0.486917E-03
  7   0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00    0.000000E 00
  8   0.000000E 00    0.000000E 00    0.206416E-02    -.169495E-03    0.205498E-02
  9   0.000000E 00    0.000000E 00    0.110018E-02    -.902805E-04    0.109524E-02

                SIMULATION HALTED AT TIME =  7200.0
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD; BEGIN SECTIONS HERE
BEGIN LAST LINE OF TEXT
3/8"
PAGE NUMBER
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
EPA-287 (Cin.)
(4-76)

```
          TOTAL CONCENTRATION OF PESTICIDE OVER TIME (PPB)
TIME(DAYS)                   COMPARTMENT NUMBER

               1       2       3       4       5       6       7       8       9
     0.0  0.0250  0.0250  0.0250  2.2500  0.0250  0.0250  0.0000  2.2500  2.2500
   600.0  0.0236  0.0153  0.0097  4.9457  0.0100  0.0069  0.0000  3.7079  2.0183
  1200.0  0.0181  0.0117  0.0074  3.8853  0.0077  0.0052  0.0000  2.9258  1.5612
  1800.0  0.0138  0.0089  0.0056  2.9697  0.0059  0.0040  0.0000  2.2379  1.1930
  2400.0  0.0105  0.0068  0.0043  2.2671  0.0045  0.0031  0.0000  1.7086  0.9108
  3000.0  0.0080  0.0052  0.0033  1.7307  0.0034  0.0023  0.0000  1.3043  0.6953
  3600.0  0.0061  0.0040  0.0025  1.3212  0.0026  0.0018  0.0000  0.9957  0.5307
  4200.0  0.0047  0.0030  0.0019  1.0085  0.0020  0.0014  0.0000  0.7601  0.4052
  4800.0  0.0036  0.0023  0.0015  0.7699  0.0015  0.0010  0.0000  0.5802  0.3093
  5400.0  0.0027  0.0018  0.0011  0.5877  0.0012  0.0008  0.0000  0.4429  0.2361
  6000.0  0.0021  0.0014  0.0009  0.4487  0.0009  0.0006  0.0000  0.3381  0.1802
  6600.0  0.0016  0.0010  0.0007  0.3425  0.0007  0.0005  0.0000  0.2581  0.1376
  7200.0  0.0012  0.0008  0.0005  0.2615  0.0005  0.0004  0.0000  0.1970  0.1050

          DISSOLVED CONCENTRATION OF PESTICIDE OVER TIME     (PPB)
TIME(DAYS)                   COMPARTMENT NUMBER

               1       2       3       4       5       6       7       8       9
     0.0  0.0099  0.0136  0.0188  0.0009  0.0125  0.0152  0.0000  0.0006  0.0008
   600.0  0.0094  0.0083  0.0073  0.0020  0.0050  0.0042  0.0000  0.0010  0.0007
  1200.0  0.0072  0.0064  0.0056  0.0016  0.0038  0.0032  0.0000  0.0008  0.0005
  1800.0  0.0055  0.0048  0.0042  0.0012  0.0029  0.0024  0.0000  0.0006  0.0004
  2400.0  0.0042  0.0037  0.0032  0.0009  0.0022  0.0019  0.0000  0.0004  0.0003
  3000.0  0.0032  0.0028  0.0025  0.0007  0.0017  0.0014  0.0000  0.0003  0.0002
  3600.0  0.0024  0.0022  0.0019  0.0005  0.0013  0.0011  0.0000  0.0003  0.0002
  4200.0  0.0019  0.0016  0.0014  0.0004  0.0010  0.0008  0.0000  0.0002  0.0001
  4800.0  0.0014  0.0013  0.0011  0.0003  0.0008  0.0006  0.0000  0.0002  0.0001
  5400.0  0.0011  0.0010  0.0008  0.0002  0.0006  0.0005  0.0000  0.0001  0.0001
  6000.0  0.0008  0.0007  0.0006  0.0002  0.0004  0.0004  0.0000  0.0001  0.0001
  6600.0  0.0006  0.0006  0.0005  0.0001  0.0003  0.0003  0.0000  0.0001  0.0000
  7200.0  0.0005  0.0004  0.0004  0.0001  0.0003  0.0002  0.0000  0.0001  0.0000
```

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA, OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
CENTER OF PAGE
TOP OF IMAGE AREA
DROPPED HEAD: BEGIN SECTIONS HERE
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

```
          PARTICULATE CONCENTRATION OF PESTICIDE OVER TIME    (PPB)
TIME(DAYS)                  COMPARTMENT NUMBER

                 1      2      3      4      5      6      7      8      9
       0.0 0.0151 0.0114 0.0062 2.2491 0.0125 0.0098 0.0000 2.2494 2.2492
     600.0 0.0142 0.0070 0.0024 4.9437 0.0050 0.0027 0.0000 3.7069 2.0176
    1200.0 0.0109 0.0054 0.0018 3.8836 0.0039 0.0021 0.0000 2.9251 1.5606
    1800.0 0.0083 0.0041 0.0014 2.9684 0.0029 0.0016 0.0000 2.2374 1.1926
    2400.0 0.0063 0.0031 0.0011 2.2662 0.0022 0.0012 0.0000 1.7082 0.9104
    3000.0 0.0048 0.0024 0.0008 1.7299 0.0017 0.0009 0.0000 1.3040 0.6950
    3600.0 0.0037 0.0018 0.0006 1.3206 0.0013 0.0007 0.0000 0.9954 0.5306
    4200.0 0.0028 0.0014 0.0005 1.0081 0.0010 0.0005 0.0000 0.7599 0.4050
    4800.0 0.0022 0.0011 0.0004 0.7696 0.0008 0.0004 0.0000 0.5801 0.3092
    5400.0 0.0016 0.0008 0.0003 0.5875 0.0006 0.0003 0.0000 0.4428 0.2360
    6000.0 0.0013 0.0006 0.0002 0.4485 0.0004 0.0002 0.0000 0.3380 0.1802
    6600.0 0.0010 0.0005 0.0002 0.3424 0.0003 0.0002 0.0000 0.2581 0.1375
    7200.0 0.0007 0.0004 0.0001 0.2613 0.0003 0.0001 0.0000 0.1970 0.1050


          MASS OF PESTICIDE ON THE MASS OF SOLIDS  (MICROGRAM PER KILOGRAM)

TIME(DAYS)                  COMPARTMENT NUMBER
       0.0     66.62     90.83    126.10      6.25     83.54    101.94      0.00      3.90      5.30
     600.0     62.91     55.64     48.74     13.73     33.53     27.94      0.00      6.42      4.76
    1200.0     48.10     42.55     37.27     10.79     25.69     21.39      0.00      5.07      3.68
    1800.0     36.72     32.48     28.45      8.25     19.61     16.33      0.00      3.88      2.81
    2400.0     28.03     24.80     21.72      6.29     14.97     12.47      0.00      2.96      2.15
    3000.0     21.40     18.93     16.58      4.81     11.43      9.52      0.00      2.26      1.64
    3600.0     16.34     14.45     12.66      3.67      8.73      7.27      0.00      1.73      1.25
    4200.0     12.47     11.03      9.66      2.80      6.66      5.55      0.00      1.32      0.96
    4800.0      9.52      8.42      7.38      2.14      5.08      4.23      0.00      1.01      0.73
    5400.0      7.27      6.43      5.63      1.63      3.88      3.23      0.00      0.77      0.56
    6000.0      5.55      4.91      4.30      1.25      2.96      2.47      0.00      0.59      0.42
    6600.0      4.24      3.75      3.28      0.95      2.26      1.88      0.00      0.45      0.32
    7200.0      3.23      2.86      2.50      0.73      1.73      1.44      0.00      0.34      0.25
OK, BO
AEGJLS (27) LOGGED OUT AT  16'35 011681
CONNECT=   24 MINUTES, CPU=  256 SECONDS, I/O=    3 SECONDS
```

DPS-307 (Cin.)
(4-79)

```
INPUT DATA FOR DIELDRIN
NUMBER OF COMPARTMENTS=   25
STEP SIZE FOR CALCULATIONS=        1.00 DAYS
TIME BETWEEN OUTPUT POINTS=      600.00 DAYS
TIME FOR SIMULATION       =     3600.00 DAYS

COMPARTMENT    INITIAL          MASS OF          PARTITION       FRACTION IN       FRACTION IN
            CONCENTRATION   SUSPENDED SOLIDS    COEFFICIENT    DISSOLVED PHASE  SUSPENDED PHASE
     1         0.0250          0.178E-02           1500.            0.272            0.728
     2         0.0250          0.156E-02           1500.            0.299            0.701
     3         0.0250          0.136E-02           1500.            0.329            0.671
     4         0.0250          0.117E-02           1500.            0.363            0.637
     5         0.0250          0.101E-02           1500.            0.398            0.602
     6         0.0250          0.700E-03           1500.            0.488            0.512
     7         0.0250          0.970E-03           1500.            0.407            0.593
     8         0.0250          0.400E-03           1500.            0.625            0.375
     9         0.0250          0.940E-03           1500.            0.415            0.585
    10         0.0250          0.240E-03           1500.            0.735            0.265
    11         0.0250          0.800E-03           1500.            0.455            0.545
    12         0.0250          0.150E-03           1500.            0.816            0.184
    13         0.0250          0.660E-03           1500.            0.503            0.497
    14         0.0250          0.900E-04           1500.            0.881            0.119
    15         0.0250          0.360E-03           1500.            0.649            0.351
    16         2.2500          0.233E 01           1500.            0.000            1.000
    17         2.2500          0.195E 01           1500.            0.000            1.000
    18         2.2500          0.163E 01           1500.            0.000            1.000
    19         2.2500          0.137E 01           1500.            0.000            1.000
    20         2.2500          0.115E 01           1500.            0.001            0.999
    21         2.2500          0.108E 01           1500.            0.001            0.999
    22         2.2500          0.102E 01           1500.            0.001            0.999
    23         2.2500          0.882E 00           1500.            0.001            0.999
    24         2.2500          0.736E 00           1500.            0.001            0.999
    25         2.2500          0.441E 00           1500.            0.002            0.998
```

Table 10. Sample output for the 30 - compartment TOXIC model

```
          PSEUCC-FIRST-ORDER RATE CONSTANTS (PER DAY)
                  IN THE DISSOLVED PHASE

 CMPN  PHOTOLYSIS   OXIDATION   HYDROLYSIS    BIOLYSIS   VOLATILIZATION
   1   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   2   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   3   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   4   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   5   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   6   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   7   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   8   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
   9   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  10   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  11   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  12   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  13   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  14   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  15   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250

OK, 0 DATA25A 1 1


  16   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  17   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  18   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  19   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  20   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  21   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  22   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  23   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  24   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
  25   0.0000000   0.0000000    0.0000000   0.0000000     0.0003250
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD: BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

```
              PSEUCC-FIRST-ORDER RATE CONSTANTS (PER DAY)
                      IN THE PARTICULATE PHASE

                  CMPN  OXIDATION   HYDROLYSIS    BIOLYSIS
                     1  0.0000000    0.0000000    0.0000000
                     2  0.0000000    0.0000000    0.0000000
                     3  0.0000000    0.0000000    0.0000000
                     4  0.0000000    0.0000000    0.0000000
                     5  0.0000000    0.0000000    0.0000000
                     6  0.0000000    0.0000000    0.0000000
                     7  0.0000000    0.0000000    0.0000000
                     8  0.0000000    0.0000000    0.0000000
                     9  0.0000000    0.0000000    0.0000000
                    10  0.0000000    0.0000000    0.0000000
                    11  0.0000000    0.0000000    0.0000000
                    12  0.0000000    0.0000000    0.0000000
                    13  0.0000000    0.0000000    0.0000000
                    14  0.0000000    0.0000000    0.0000000
                    15  0.0000000    0.0000000    0.0000000
                    16  0.0026000    0.0000000    0.0000000
                    17  0.0026000    0.0000000    0.0000000
                    18  0.0026000    0.0000000    0.0000000
                    19  0.0026000    0.0000000    0.0000000
                    20  0.0026000    0.0000000    0.0000000
                    21  0.0026000    0.0000000    0.0000000
                    22  0.0026000    0.0000000    0.0000000
                    23  0.0026000    0.0000000    0.0000000
                    24  0.0026000    0.0000000    0.0000000
                    25  0.0026000    0.0000000    0.0000000

 DO YOU WANT AN ECHO CHECK OF THE INPUT DATA? (1=YES,2=NO)
2

DO YOU WANT INTERMEDIATE OUTPUT (1=YES),(2=NO) ?
2

         INPUT: CIN(1)=0.15*EXP(-0.00045*TIM)
```

```
                   TIME=   600.0 DAYS

 0.89363E-01   0.70278E-01   0.55779E-01   0.44737E-01   0.36282E-01
 0.29454E-01   0.29568E-01   0.22220E-01   0.25350E-01   0.18133E-01
 0.20735E-01   0.15647E-01   0.16819E-01   0.14143E-01   0.14342E-01
 0.19820E 02   0.14974E 02   0.11382E 02   0.86935E 01   0.67113E 01


OK, 0 DATA25A 1 1


 0.54061E 01   0.46062E 01   0.35868E 01   0.27446E 01   0.18043E 01
      VOL=        1.23             AL=        1.050


                   TIME= 1200.0 DAYS
 0.68719E-01   0.54426E-01   0.43490E-01   0.35101E-01   0.28632E-01
 0.23254E-01   0.23546E-01   0.17566E-01   0.20316E-01   0.14359E-01
 0.16693E-01   0.12413E-01   0.13577E-01   0.11231E-01   0.11492E-01
 0.18207E 02   0.13845E 02   0.10568E 02   0.80823E 01   0.62274E 01
 0.50245E 01   0.42736E 01   0.32797E 01   0.24450E 01   0.14886E 01
      VOL=        1.23             AL=        1.050
```

```
                    TIME= 1800.0 DAYS

0.52543E-01    0.41684E-01    0.33363E-01    0.26972E-01    0.22036E-01
0.17899E-01    0.18170E-01    0.13526E-01    0.15709E-01    0.11063E-01
0.12928E-01    0.95691E-02    0.10527E-01    0.86611E-02    0.88906E-02
0.14421E 02    0.11004E 02    0.84261E 01    0.64607E 01    0.49872E 01
0.40393E 01    0.34437E 01    0.26416E 01    0.19631E 01    0.11753E 01

     VOL=        1.23            AL=        1.050


                    TIME= 2400.0 DAYS

0.40125E-01    0.31844E-01    0.25498E-01    0.20622E-01    0.16855E-01
0.13651E-01    0.13909E-01    0.10348E-01    0.12032E-01    0.84648E-02
0.99076E-02    0.73232E-02    0.80712E-02    0.66291E-02    0.68120E-02
0.11097E 02    0.84789E 01    0.65003E 01    0.49895E 01    0.38552E 01
0.31281E 01    0.26701E 01    0.20494E 01    0.15229E 01    0.90793E 00

     VOL=        1.23            AL=        1.050


                    TIME= 3000.0 DAYS

0.30633E-01    0.24314E-01    0.19470E-01    0.15745E-01    0.12873E-01
0.10457E-01    0.10625E-01    0.79036E-02    0.91936E-02    0.64656E-02
0.75713E-02    0.55940E-02    0.61688E-02    0.50639E-02    0.52054E-02
0.84864E 01    0.64867E 01    0.49749E 01    0.38201E 01    0.29527E 01
0.23974E 01    0.20474E 01    0.15720E 01    0.11683E 01    0.69577E 00

     VOL=        1.23            AL=        1.050
```

```
                      TIME= 3600.0 DAYS

OK, 0 DATA25A 1 1



  0.23385E-01    0.18561E-01    0.14864E-01    0.12023E-01    0.98285E-02
  0.79837E-02    0.81127E-02    0.60343E-02    0.70198E-02    0.49365E-02
  0.57814E-02    0.42710E-02    0.47107E-02    0.38664E-02    0.39748E-02
  0.64809E 01    0.49543E 01    0.38001E 01    0.29183E 01    0.22560E 01
  0.18321E 01    0.15649E 01    0.12017E 01    0.89320E 00    0.53175E 00
        VOL=          1.23               AL=        1.050


                 SIMULATION HALTED AT TIME =  3600.0


          TOTAL CONCENTRATION OF PESTICIDE OVER TIME (PPB)
                          COMPARTMENT NUMBER
        1
        6               2              3
       11               7              8              4              5
       16              12             13              9             10
       21              17             18             14             15
                       22             23             19             20
                                                      24             25

                      TIME=     0.0 DAYS
  0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01
  0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01
  0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01    0.25000E-01
  0.22500E 01    0.22500E 01    0.22500E 01    0.22500E 01    0.22500E 01
  0.22500E 01    0.22500E 01    0.22500E 01    0.22500E 01    0.22500E 01
```

BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
CENTER OF PAGE
TOP OF IMAGE AREA
EPA-287 (Cin.) (6-76)

```
                         TIME=  600.0 DAYS
 0.89363E-01   0.70278E-01   0.55779E-01   0.44737E-01   0.36282E-01
 0.29454E-01   0.29568E-01   0.22220E-01   0.25350E-01   0.18133E-01
 0.20735E-01   0.15647E-01   0.16819E-01   0.14143E-01   0.14342E-01
 0.19820E 02   0.14974E 02   0.11382E 02   0.86935E 01   0.67113E 01
 0.54061E 01   0.46062E 01   0.35868E 01   0.27446E 01   0.18043E 01

                         TIME= 1200.0 DAYS
 0.68719E-01   0.54426E-01   0.43490E-01   0.35101E-01   0.28632E-01
 0.23254E-01   0.23546E-01   0.17566E-01   0.20316E-01   0.14359E-01
 0.16693E-01   0.12413E-01   0.13577E-01   0.11231E-01   0.11492E-01
 0.18207E 02   0.13845E 02   0.10568E 02   0.80823E 01   0.62274E 01
 0.50245E 01   0.42736E 01   0.32797E 01   0.24450E 01   0.14886E 01

                         TIME= 1800.0 DAYS
 0.52543E-01   0.41684E-01   0.33363E-01   0.26972E-01   0.22036E-01
 0.17899E-01   0.18170E-01   0.13526E-01   0.15709E-01   0.11063E-01
 0.12928E-01   0.95691E-02   0.10527E-01   0.86611E-02   0.88906E-02
 0.14421E 02   0.11004E 02   0.84261E 01   0.64607E 01   0.49872E 01
 0.40393E 01   0.34437E 01   0.26416E 01   0.19631E 01   0.11753E 01

OK, C CATA25A 1 1

                         TIME= 2400.0 DAYS
 0.40125E-01   0.31844E-01   0.25498E-01   0.20622E-01   0.16855E-01
 0.13651E-01   0.13909E-01   0.10348E-01   0.12032E-01   0.84648E-02
 0.99076E-02   0.73232E-02   0.80712E-02   0.66291E-02   0.68120E-02
 0.11097E 02   0.84789E 01   0.65003E 01   0.49895E 01   0.38552E 01
 0.31281E 01   0.26701E 01   0.20494E 01   0.15229E 01   0.90793E 00
```

```
                     TIME= 3000.0 DAYS

  0.30633E-01   0.24314E-01   0.19470E-01   0.15749E-01   0.12873E-01
  0.10457E-01   0.10625E-01   0.79036E-02   0.91936E-02   0.64656E-02
  0.75713E-02   0.55940E-02   0.61688E-02   0.50639E-02   0.52054E-02
  0.84864E 01   0.64867E 01   0.49749E 01   0.38201E 01   0.29527E 01
  0.23974E 01   0.20474E 01   0.15720E 01   0.11683E 01   0.69577E 00


                     TIME= 3600.0 DAYS

  0.23385E-01   0.18561E-01   0.14864E-01   0.12023E-01   0.98285E-02
  0.79837E-02   0.81127E-02   0.60343E-02   0.70198E-02   0.49365E-02
  0.57814E-02   0.42710E-02   0.47107E-02   0.38664E-02   0.39748E-02
  0.64809E 01   0.49543E 01   0.38001E 01   0.29183E 01   0.22560E 01
  0.18321E 01   0.15649E 01   0.12017E 01   0.89320E 00   0.53175E 00



        DISSOLVED CONCENTRATION OF PESTICIDE OVER TIME      (PPB)

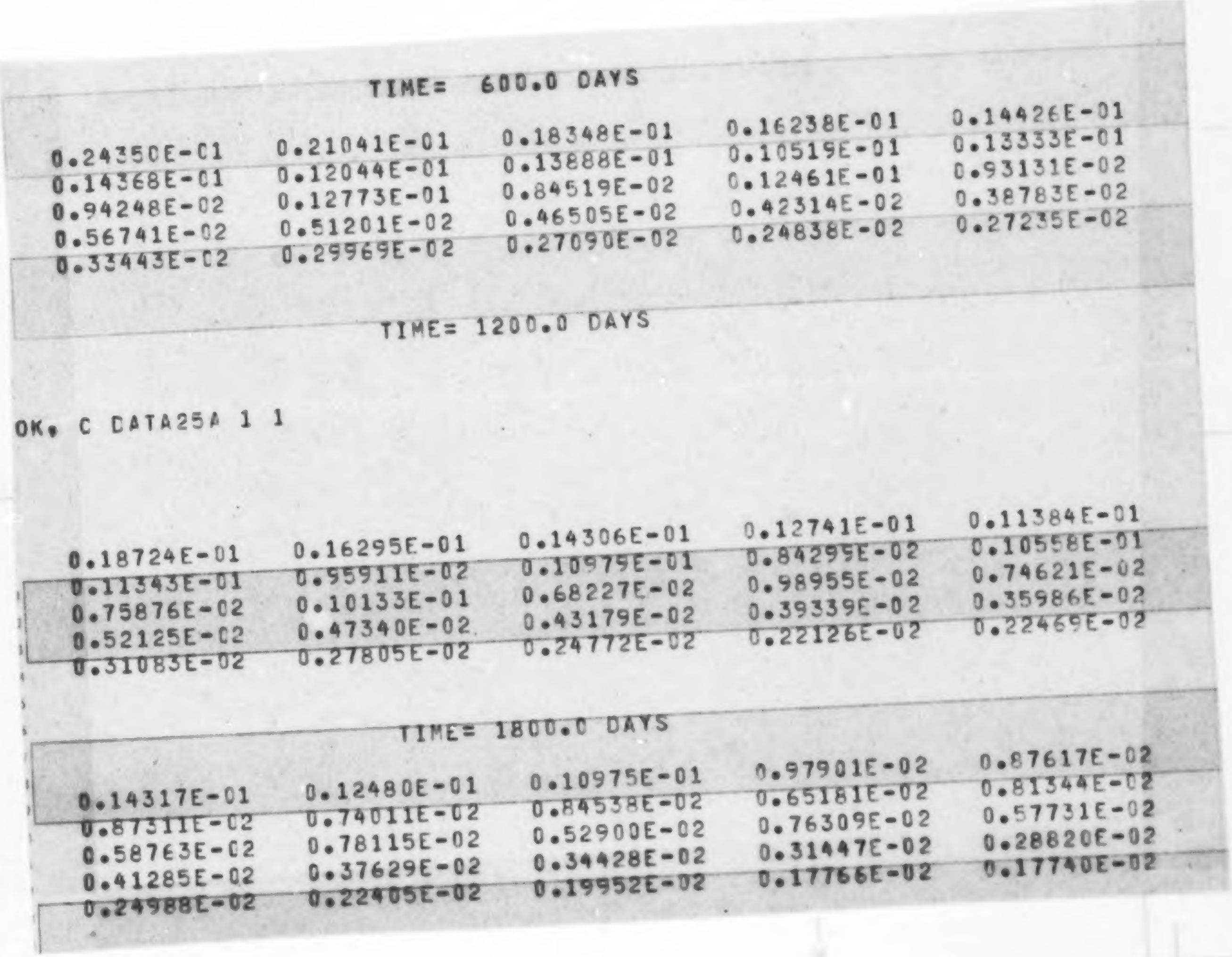
                       COMPARTMENT NUMBER

       1             2             3             4             5
       6             7             8             9            10
      11            12            13            14            15
      16            17            18            19            20
      21            22            23            24            25


                     TIME=     0.0 DAYS

  0.68120E-02   0.74850E-02   0.82237E-02   0.90744E-02   0.99404E-02
  0.12195E-01   0.10183E-01   0.15625E-01   0.10373E-01   0.18382E-01
  0.11364E-01   0.20408E-01   0.12563E-01   0.22026E-01   0.16234E-01
  0.64415E-03   0.76936E-03   0.91931E-03   0.10952E-02   0.13002E-02
  0.13919E-02   0.14639E-02   0.16994E-02   0.20362E-02   0.33962E-02
```

BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA: OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-76)



```
                        TIME=  600.0 DAYS

  0.24350E-01   0.21041E-01   0.18348E-01   0.16238E-01   0.14426E-01
  0.14368E-01   0.12044E-01   0.13888E-01   0.10519E-01   0.13333E-01
  0.94248E-02   0.12773E-01   0.84519E-02   0.12461E-01   0.93131E-02
  0.56741E-02   0.51201E-02   0.46505E-02   0.42314E-02   0.38783E-02
  0.33443E-02   0.29969E-02   0.27090E-02   0.24838E-02   0.27235E-02

                        TIME= 1200.0 DAYS

OK, C DATA25A 1 1


  0.18724E-01   0.16295E-01   0.14306E-01   0.12741E-01   0.11384E-01
  0.11343E-01   0.95911E-02   0.10979E-01   0.84295E-02   0.10558E-01
  0.75876E-02   0.10133E-01   0.68227E-02   0.98955E-02   0.74621E-02
  0.52125E-02   0.47340E-02   0.43179E-02   0.39339E-02   0.35986E-02
  0.31083E-02   0.27805E-02   0.24772E-02   0.22126E-02   0.22469E-02

                        TIME= 1800.0 DAYS

  0.14317E-01   0.12480E-01   0.10975E-01   0.97901E-02   0.87617E-02
  0.87311E-02   0.74011E-02   0.84538E-02   0.65181E-02   0.81344E-02
  0.58763E-02   0.78115E-02   0.52900E-02   0.76309E-02   0.57731E-02
  0.41285E-02   0.37629E-02   0.34428E-02   0.31447E-02   0.28820E-02
  0.24988E-02   0.22405E-02   0.19952E-02   0.17766E-02   0.17740E-02
```

```
                         TIME= 2400.0 DAYS

  0.10933E-01    0.95342E-02    0.83876E-02    0.74854E-02    0.67019E-02
  0.66788E-02    0.56656E-02    0.64674E-02    0.49927E-02    0.62241E-02
  0.45034E-02    0.59781E-02    0.40559E-02    0.58406E-02    0.44234E-02
  0.31770E-02    0.28993E-02    0.26559E-02    0.24286E-02    0.22278E-02
  0.19351E-02    0.17372E-02    0.15479E-02    0.13782E-02    0.13705E-02


                         TIME= 3000.0 DAYS

  0.83468E-02    0.72795E-02    0.64047E-02    0.57164E-02    0.51187E-02
  0.51010E-02    0.43280E-02    0.49398E-02    0.38148E-02    0.47541E-02
  0.34415E-02    0.45665E-02    0.30999E-02    0.44616E-02    0.33802E-02
  0.24295E-02    0.22181E-02    0.20326E-02    0.18594E-02    0.17063E-02
  0.14831E-02    0.13321E-02    0.11873E-02    0.10573E-02    0.10502E-02


                         TIME= 3600.0 DAYS

  0.63719E-02    0.55572E-02    0.48895E-02    0.43642E-02    0.39080E-02
  0.38545E-02    0.33045E-02    0.37714E-02    0.29128E-02    0.36298E-02
  0.26279E-02    0.34866E-02    0.23672E-02    0.34065E-02    0.25810E-02
  0.18554E-02    0.16941E-02    0.15526E-02    0.14205E-02    0.13037E-02
  0.11334E-02    0.10182E-02    0.90763E-03    0.80833E-03    0.80265E-03


       PARTICULATE CONCENTRATION OF PESTICIDE OVER TIME    (PPB)

                      COMPARTMENT NUMBER

      1              2              3              4              5
      6              7              8              9             10
     11             12             13             14             15
     16             17             18             19             20
     21             22             23             24             25
```

TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA: OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER
EPA-287 (Cin.)
(4-76)

```
                        TIME=     0.0 DAYS
  0.18188E-01    0.17515E-01    0.16776E-01    0.15926E-01    0.15060E-01
  0.12805E-01    0.14817E-01    0.93750E-02    0.14627E-01    0.66176E-02

OK, 0 DATA25A 1 1


  0.13636E-01    0.45918E-02    0.12437E-01    0.29736E-02    0.87662E-02
  0.22494E 01    0.22492E 01    0.22491E 01    0.22489E 01    0.22487E 01
  0.22486E 01    0.22485E 01    0.22483E 01    0.22480E 01    0.22466E 01

                        TIME=   600.0 DAYS
  0.65013E-01    0.49236E-01    0.37431E-01    0.28498E-01    0.21855E-01
  0.15086E-01    0.17524E-01    0.83326E-02    0.14831E-01    0.47998E-02
  0.11310E-01    0.28739E-02    0.83674E-02    0.16822E-02    0.50291E-02
  0.19814E 02    0.14969E 02    0.11377E 02    0.86892E 01    0.67074E 01
  0.54028E 01    0.46032E 01    0.35841E 01    0.27422E 01    0.18016E 01

                        TIME=  1200.0 DAYS
  0.45994E-01    0.38131E-01    0.29184E-01    0.22360E-01    0.17247E-01
  0.11910E-01    0.13955E-01    0.65872E-02    0.11886E-01    0.38010E-02
  0.91052E-02    0.22800E-02    0.67544E-02    0.13359E-02    0.40256E-02
  0.18202E 02    0.13840E 02    0.10564E 02    0.80783E 01    0.62238E 01
  0.50214E 01    0.42709E 01    0.32773E 01    0.24427E 01    0.14863E 01

                        TIME=  1800.0 DAYS
  0.38226E-01    0.29204E-01    0.22388E-01    0.17182E-01    0.13274E-01
  0.91676E-02    0.10769E-01    0.50723E-02    0.91905E-02    0.29284E-02
  0.70515E-02    0.17576E-02    0.52371E-02    0.10302E-02    0.31175E-02
  0.14417E 02    0.11001E 02    0.84227E 01    0.64576E 01    0.49844E 01
  0.40368E 01    0.34414E 01    0.26396E 01    0.19613E 01    0.11735E 01
```

```
                                TIME= 2400.0 DAYS

  0.29192E-01     0.22310E-01     0.17111E-01     0.13137E-01     0.10153E-01
  0.70127E-02     0.82434E-02     0.38805E-02     0.70397E-02     0.22407E-02
  0.54041E-02     0.13451E-02     0.40153E-02     0.78848E-03     0.23886E-02
  0.11054E 02     0.84760E 01     0.64976E 01     0.49870E 01     0.38530E 01
  0.31262E 01     0.26684E 01     0.20479E 01     0.15215E 01     0.90656E 00

                                TIME= 3000.0 DAYS

  0.22286E-01     0.17034E-01     0.13066E-01     0.10032E-01     0.77548E-02
  0.53561E-02     0.62973E-02     0.29639E-02     0.53788E-02     0.17115E-02
  0.41298E-02     0.10275E-02     0.30689E-02     0.60232E-03     0.18253E-02
  0.84839E 01     0.64845E 01     0.49729E 01     0.38182E 01     0.29510E 01
  0.23959E 01     0.20461E 01     0.15708E 01     0.11673E 01     0.69472E 00

                                TIME= 3600.0 DAYS

  0.17013E-01     0.13004E-01     0.99746E-02     0.76591E-02     0.59206E-02
  0.40892E-02     0.48081E-02     0.22629E-02     0.41070E-02     0.13067E-02
  0.31535E-02     0.78447E-03     0.23435E-02     0.45988E-03     0.13938E-02
  0.64791E 01     0.49526E 01     0.37985E 01     0.29169E 01     0.22547E 01
  0.18309E 01     0.15639E 01     0.12008E 01     0.89239E 00     0.53095E 00
```

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

EPA-287 (Cin.)
(4-76)

```
OK, C DATA25A 1 1


        MASS OF PESTICIDE ON THE MASS OF SOLIDS  (MICROGRAM PER KILOGRAM)

                            COMPARTMENT NUMBER
      1               2               3               4               5
      6               7               8               9              10
     11              12              13              14              15
     16              17              18              19              20
     21              22              23              24              25

                      TIME=     0.0 DAYS
      10.22           11.23           12.34           13.61           14.91
      18.29           15.27           23.44           15.56           27.57
      17.05           30.61           18.84           33.04           24.35
       0.97            1.15            1.38            1.64            1.95
       2.09            2.20            2.55            3.05            5.09

                      TIME=   600.0 DAYS
      36.52           31.56           27.52           24.36           21.64
      21.55           18.07           20.83           15.78           20.00
      14.14           19.16           12.68           18.69           13.97
       8.51            7.68            6.98            6.35            5.82
       5.02            4.50            4.06            3.73            4.09

                      TIME= 1200.0 DAYS
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BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER
EPA-287 (Cin.)
(4-78)

```
     28.09          24.44          21.46          19.11          17.08
     17.01          14.39          16.47          12.64          15.84
     11.38          15.20          10.23          14.84          11.19
      7.82           7.10           6.48           5.90           5.40
      4.66           4.17           3.72           3.32           3.37

              TIME= 1800.0 DAYS
     21.48          18.72          16.46          14.69          13.14
     13.10          11.10          12.68           9.78          12.20
      8.81          11.72           7.93          11.45           8.66
      6.15           5.64           5.16           4.72           4.32
      3.75           3.36           2.99           2.66           2.66

              TIME= 2400.0 DAYS
     16.40          14.30          12.58          11.23          10.05
     10.02           8.50           9.70           7.49           9.34
      6.76           8.97           6.08           8.76           6.64
      4.77           4.35           3.98           3.64           3.34
      2.90           2.61           2.32           2.07           2.06

              TIME= 3000.0 DAYS
     12.52          10.92           9.61           8.57           7.68
```

EPA-287 (Cin.)
(4-76)

```
OK, O DATA25A 1 1


            7.65          6.49          7.41          5.72          7.13
            5.16          6.85          4.65          6.69          5.07
            3.64          3.33          3.05          2.79          2.56
            2.22          2.00          1.78          1.59          1.58

                   TIME= 3600.0 DAYS

            9.56          8.34          7.33          6.55          5.86
            5.84          4.96          5.66          4.37          5.44
            3.94          5.23          3.55          5.11          3.87
            2.78          2.54          2.33          2.13          1.96
            1.70          1.53          1.36          1.21          1.20

OK, COMO -E
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TYPING GUIDE SHEET
BEGIN FIRST LINE OF TEXT HERE
DROPPED HEAD. BEGIN SECTIONS HERE
CENTER OF PAGE
TOP OF IMAGE AREA
BEGIN LAST LINE OF TEXT
3/8"
BOTTOM OF IMAGE AREA; OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
PAGE NUMBER